LA-UR-05-7263

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Title:

Symposium on Modeling & Simulation of Variable Density & Compressible Turbulent Mixing Summary Report

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September 23, 2005

Abstract

This report summarizes the proceedings for the technical sessions of a workshop on modeling and simulation of turbulent mixing in variable density/compressible flows held August 3-5, 2005 in Los Alamos. The goal of the workshop was to foster a dialogue between researchers working on fundamental turbulence issues, numerical simulation, and modeling of variable density and compressible turbulent mixing. In order to accomplish this goal, the workshop brought together experts from national laboratories (Los Alamos, Lawrence Livermore, and Sandia), industry, and academia to explore the extension of state-of-the-art turbulence modeling approaches to applications of interest to the Los Alamos National Laboratory and the DOE. Approximately 70 people attended the symposium which consisted of 20 invited talks in the first two days of the meeting. The technical talks were followed by “second-chances”, whereby speakers were given the opportunity to clarify or expand on important points from their talks, and open round-table discussions. The diverse cross-section of speakers permitted a broad sampling of advanced numerical methods, physical insight related to the applications of interest, and modern modeling approaches as the basis for answering the question “How can advanced turbulence modeling approaches be used/extended for lab-centric applications?” The symposium provided a unique opportunity to survey state-of-the-art approaches to turbulence modeling that ranged from moment closures to Large Eddy Simulations based on explicit stochastic and deterministic physical subgrid models, implicit LES, the compressible Lagrangian averaging Navier-Stokes equations, variational multiscale and hybrid approaches. The issues associated with multi-fluid simulations, e.g., the importance of interface physics, were also addressed. This symposium marks the first-step in a focused effort to advance the modeling and simulation capabilities for compressible turbulent mixing at Los Alamos National Laboratory.

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Summary of Findings

The purpose for this section is to provide a synopsis of the key issues raised during the first two days of the symposium. The issues identified here come directly from notes taken during discussion immediately following talks, in the second-chances sessions, and during the round-tables. The detailed transcripts may be found in the section entitled "Abstracts and Discussion Highlights".

Physical Insights and Modeling Issues

- In the context of shock-accelerated flows, the secondary baroclinic circulation is much greater than the primary (deposited by the shock) due to vortex acceleration and gradient intensification of the transition layer. Therefore, it is critically important to accurately capture the baroclinic gradient intensification process.
  - Recognized need to look at both structure and growth of the mixing layer
  - Enstrophy as an indicator of the mixing layer structure
- Euler equations don't exhibit pointwise convergence, and in multi-dimensions may be ill-posed. Small scale-structures in simulations using the Euler equations are set by the regularizing (artificial) viscosity.
- The amount of diffusion at the interface between fluids is very important for capturing the evolution of the flow.
- Stable numerical methods require some damping at the grid Nyquist limit ($2\Delta x$), and believable results are probably represented at 4 or 8 Δx. Accurate modeling may require integration at these wavelengths rather than at the Nyquist limit.
  - There is a clear need to distinguish between what is numerics and what is physics.
- "Noise", consisting of fluctuations at or below the grid-scale, can affect the evolution of the large-scale (resolvable) flow features. Representing the effects of sub-grid scale fluctuations poses problems for coarse-grid computations, e.g., in LES.
- Hybrid LES-RANS approaches may be a viable approach for certain coupled multiphysics applications where there is a need to capture the effects of coupled, time-dependent phenomena in the face of finite computing resources.

Scale-Breaking Phenomena

- Scale-breaking phenomena consist of effects due to surface tension and mass diffusion at interfaces, compressibility, long wavelength perturbations, etc. These effects can be physical or introduced by numerical artifacts, e.g., numerical surface tension in interface tracking.
- Scale-breaking phenomena in acceleration-driven mixing (e.g., Rayleigh-Taylor and Richtmeyer-Meshkov flows) can result in important and observable macroscopic changes.
- The impact of scale-breaking phenomena on the growth of the mixing layer is important, and perhaps has not been considered adequately.

Large-Eddy Simulation

- Implicit LES (ILES) has made progress, but not all implicit SGS modeling approaches work. For example, the case of temperature-dependent viscosity still poses problems for ILES approaches. In general, ILES may not be suitable for flows where important physics occur at the small scales, e.g., in non-premixed combustion. In this case the algorithm should be supplemented with an explicit subgrid model.

- The representation of "noise", i.e., subgrid-scale or grid-scale fluctuations may be difficult to represent adequately in LES with simple closure models.
- The CLANS-alpha model may be interpreted as a compressible LES, and the solution of the global Helmholtz equation introduced in the alpha model can be viewed as the global inversion of a local filter.
- Filters and sub-filter modeling may provide a more useful conceptual framework than subgrid models.
- Most LES are based on a filter independent of the flow features, but typically tied to the grid Nyquist limit. Filtering in terms of the most energetic structures may be a more suitable approach.
- There is a need for the LES community to compare the predictions to well-established "canonical" problems, e.g., Compte-Bellot and Corrsin experiment.
- RANS attempts to evolve the statistics of an ensemble average and is good for representing behavior in the mean. LES may be more appropriate for investigating point excursions from mean behavior.
- Some open issues
    - What is required for an explicit filter for complex geometry and unstructured grids?
    - What is the best filter/filtering approach for LES when the turbulence is inhomogeneous?
    - What are the errors associated with applying the SGS model at the grid Nyquist limit?
    - What are the relationships between the mesh and filter scales?
    - What statistics should LES predict? Should they be spatial or temporal statistics?
    - How should backscatter be represented?
- Notable quotations

  "LES started out being about the large scales, but turbulence is about more than the large scales"
  Dale Pullin, CalTech

  "Put life into the subgrid scale …" Darryl Holm, Los Alamos National Laboratory

Numerics/Computational Issues

- Criteria are needed to assess whether a given numerical simulation is sufficiently accurate for performing compressible/variable density turbulence simulations.
- In the discussion of numerical accuracy, the treatment of interfaces is far more important than the order of accuracy of a given method. As demonstrated by Rider and Kothe, untracked methods are the worst, and there is a hierarchy among the interface methods in terms of accuracy.
- The use of LES with AMR poses challenges in terms of the time-integration and error control at the interface between different meshes, but appears tractable.

Abstracts and Discussion Highlights

This section presents the abstract for each speaker in the unclassified sessions, and highlights the primary points of each talk, and question/answer segment that followed each talk. A detailed transcript of the discussion during the "second chances" segment and the round-table sessions are presented in the ensuing sections. Every attempt was made to associate specific attendees with questions and comments in order to provide a coherent transcript of the rich discussion that occurred on each day of the workshop. A brief list of technical abbreviations is provided below to assist the reader in understanding the technical details of the discussion where abbreviations in the transcribed highlights were made.

Nomenclature:

CLANS	Compressible Lagrangian-Averaged Navier-Stokes
CLES	Compressible LES
CVS	Coherent Vortex Simulation
DNS	Direct Numerical Simulation
EP	Euler-Poincare'
FCT	Flux-Corrected Transport
FDV	Fully-Developed Turbulence
GLM	Generalized Lagrangian Mean
GMRES	Generalized Minimum Residual
ILES	Implicit LES
ILU	Incomplete LU (factorization)
KH	Kelvin-Helmholtz
LES	Large-Eddy Simulation
LGB	Locally Grid-Based
MILES	Monotonically Integrated LES
NURBS	Non-Uniform Rational B-Spline
ODE	Ordinary Differential Equation
ODT	One-Dimensional Turbulence
NFV	Nodal Finite-Volume
PDF	Probability Distribution Function
PLIF	Particle-Laser Interferometry
PPM	Piecewise Parabolic Method
PW	Pratt-Whitney
RANS	Reynolds-Averaged Navier-Stokes
RM	Richtmyer-Meshkov
RT	Rayleigh-Taylor
SAMR	Structured Adaptive Mesh Refinement
SGS	SubGrid-Scale
SF6	Sulfur-Hexaflouride
TCD	Tuned Central-Difference
VBL	Vorticity Bilayers
WENO	Weighted Essentially Non-Oscillatory

Wednesday, August 3, 2005

Daniel Livescu, Los Alamos National Laboratory, *Opening Remarks*

This symposium is designed to encourage a dialogue on turbulent mixing as occurs in Rayleigh-Taylor and Richtmyer-Meshkov instabilities. We tried to have as many perspectives as possible to ensure a constructive dialog. Trying to simulate complex flows like Richtmyer-Meshkov or Rayleigh-Taylor instabilities at high Reynolds numbers poses difficult challenges. There are clear numerical issues when dealing with these flows, e.g. in handling shock waves or interfaces. There is also a turbulence modeling issue since the flows are anisotropic and non-homogeneous and a model should capture the whole evolution of the flow from laminar, through transition, and to the fully turbulent regime. Finally, turbulence in these conditions or in even simpler situations involving variable density or compressibility effects is also an important theoretical problem and its better understanding can lead to improved models and requirements for numerical approaches.

Norman Zabusky, Rutgers University, *Vorticity Deposition and Evolution in Shock Accelerated Flows: Analysis, Computation and Experiment*

This talk presents an overview and recent understanding of accelerated inhomogeneous flows or shock-accelerated Richtmyer-Meshkov flows. We use the vortex paradigm and the visiometrics approach. We project data to lower dimensions to quantify, validate simulations of and model phenomena involving coherent space-time events. We emphasize our recent work, including vortex induced secondary baroclinic circulation generation, which yields more positive and negative circulation through intermediate times than the original shock-accelerated vortex deposition. We apply this to the one mode classical configuration and the shock cylinder. In addition we quantify the effects of the initial thickness of the interfacial transition layer and the ubiquity of "vortex projectiles" and transition to baroclinic turbulence.

- Our objectives are to understand and model vortex physics and mixing. The approach we use involves simulation, visiometrics, juxtaposition and modeling. I will discuss how one might visualize the flow. I will show several experiments in my talk. I will emphasize some key points:
  - The generation of vortex bilayers and the gradient intensification that is associated with this.
  - What is the amplitude rate of change in RM at intermediate times?
  - Vortex projectiles (dipoles & rings)
  - I will not discuss algorithms (we use PPM in two versions and the FLASH code)
  - Showed "typical" Rayleigh-Taylor equations with interfacial shear and surface tension.
  - Showed geometries studied over past few years including curtain, shock cylinder and shock ellipse)
  - Discussed baroclinic equation for vorticity in three dimensions. There are two important things to keep in mind – (1) The gradient of rho (ρ) is the essence in this equation and (2) the transition layer in the density interface must be treated properly.
  - (Showed pictures from the Jacobs and Niederhaus 2003 Dropped Tank Experiment). One must be careful of secondary structures when looking at the rollups. The solution exists

only for a finite time. Discussed Rayleigh-Taylor (RT) & Richtmyer-Meshkov (RM) Finite Time singularity – the scale is governed by the grid size. As the grid size grows smaller the structure becomes smaller. Putting in a thicker, more realistic transition layer or adding viscosity can help to overcome this. Showed ten year old picture of RM planar inclined interface (goal of calculation was to seek agreement with experimental data).

- How should we view this complex of information? We introduce the idea of space-time diagram.
- We are conscious of circulation generation and rate of circulation generation and have developed a new diagnostic. By carefully selecting key places in the domain we can pick out both the positive and negative circulation.
- The gradient of the interface is intensifying. As time proceeds the gradient increases and the number of points that have gradients is increasing. We do not understand the fundamentals of this but believe that it is of the essence to developing turbulence.
- Looking at vortex-accelerated "secondary" baroclinic vorticity deposition – initially one side of the domain has all of one sign vorticity and as it rolls up it begins to generate the other sign – it grows more complex. (Showed pictures with intensifying interface and large region of positive vorticity). The secondary rollup is not a simple Kelvin-Helmholtz (KH) instability. [Showed Vizlab simulations (PPM) of G. Peng and S. Zhang and Jacob and Krivet's Experiment (PLIF)]. How to talk about agreement? Discussed global quantifications of circulation. It is critically important to get the baroclinic gradient intensification process correct.
- Good experimental agreement is an important issue. In the past few years the experiments have gotten much better and we can get more information from them. When the LANL group presented some experimental results at the APS meeting we were impressed with what we heard and decided to focus on the interface transition layer issue. (Showed a comparison of LANL experimental issues and a simulation with visiometrics). What is known about the initial conditions? It is hard to deduce the density gradient. One can see at which point the laminar begins to show perturbations on the interface and then the vortices. Our simulation characterizes the bounding box and shows good agreement up to a certain point. We see that two different initial conditions for the Jacobs' Experiment generate two (somewhat) different vorticity dispositions. We have a qualitative agreement.
- Velocity magnitude distribution is a very sensitive issue. We can obtain very good agreement but there is more work to be done.
- At a certain time (there are five times in the shock curtain experiment) one gets an initial behavior (showed power spectrum in 2D calculation).
- Secondary Baroclinic Circulation is much greater than the primary (deposited by shock) due to vortex acceleration and gradient intensification of the transition layer. A new diagnostic is the rate of change of circulation in bubble to spike domain.

Question – How would you visualize energy generated at large scales?

- The forces are being generated at the scale of the Baroclinic process. If there is no mechanism to prevent the gradients from not steeping, the diffusivity of the code is important.

Pullin – Is there a local Reynolds number that can help to organize transitions from stability to instability?

- I do not think it is the intrinsic Reynolds's number but the dissipative change. Is it the intrinsic dissipation of the medium in the 3D sense or the thickness of the cell? I think it is the latter.

Pullin – If you go to 3D would you expect the secondary Baroclinic instabilities to be happening on a small scale?

- The proper response to that question has many components. I do not believe I can competently answer that question for 3D. For 2D the vorticity is being deposited regardless of cell size. I do not understand how this translates into power spectra (it has not been looked at the - to best of my knowledge).

Shuang Zhang, Fluent, *Turbulent Decay and Mixing of Accelerated Inhomogeneous Flows via Flow Feature Analysis*

We review our work on the laminar and turbulent evolution of accelerated inhomogeneous flow environments – generalizations of the basic Richtmyer-Meshkov configurations. We have simulated numerically the 2D and 3D compressible Euler equations, where a shock wave interacts with a gas layer (curtain).

We observed and quantify many generic phenomena in the shock accelerated inhomogeneous flows, e.g., the generation of vortex projectiles and decay of unforced turbulent states. In addition, scaling laws are developed for variations of circulation and enstrophy with Mach and Atwood numbers, particularly, the unusual strong monotonic growth of positive and negative circulation by secondary baroclinic processes. Energy and enstrophy decay and power spectra are examined to late-intermediate times. Although the intrinsic numerical dissipation causes our decaying turbulence, we observe excellent agreement with previous work on 2D viscous isotropic homogeneous turbulence in the inertial range. Note that the baroclinic circulation generation in this environment plays a major role in the mass transport and mixing. The mass-transport induced density gradient intensification enhances the circulation generation and provides an intrinsic forcing at intermediate to high wave number range. 3D simulations also exhibit strong enstrophy growth at intermediate times.

The flow feature extraction and tracking analysis framework provides a powerful tool for synergizing flow visualization with the flow physics. We study and compare light curtain (slow/fast/slow) with heavy curtain (fast/slow/fast) configurations to illustrate heuristically the correlations of mass and momentum diffusivity, and to address quantitatively the spatial and temporal diffusivity of the mixing zone. We will also report the current status of building more intense mining of flow features and PDE solution procedure.

- I will discuss 2D shock curtain simulation with the emergence of vorticity bilayers (VBL) and random vortex projectiles, strong secondary baroclinic circulation deposition. I will also discuss a 3D shock-curtain simulation with vortex feature identification, applications and challenges. We will discuss three simulations – the 3D simulation involves a heavy curtain case.
- (Showed current geometry: computation domain, Euler, PPM simulation. Showed movie of vorticity field of 2D light curtain simulation followed by detail in static pictures).

- First we take data transformation and extract the feature of interest, then we track the feature over time and isolate the feature (in an interactive manner) and quantify it. (Showed 2D feature extraction results of late time image). We see interesting differences between light and heavy curtain cases. For the heavy curtain case the vortex is outside of the material. Average density variation indicates mass diffusion – in the heavy case this decreases, in the light case this increases. We see the mixing rate for the heavy curtain mass diffuses at a higher rate. If we correlate this with the momentum of the vortex feature we find the average vorticity indicates momentum diffusion for both cases.
- The main vortex concentration is coincident with low density so in the heavy curtain mass the vortex structures are outside heavy materials structures and cause a more rapid mass diffusion, which serves as a momentum source.
- For 3D accurate identification of the vortex structure is critical. (Showed simulation of 3D SF6 vortex circulation in air). [Discussed problems associated with existing physics methods (pressure minimum region, λ_2, vorticity magnitude, helicity)].
  - Note: λ_2 is the second eigenvalue of the strain-rate, $\frac{1}{2}\left(\partial u_i/\partial x_j + \partial u_j/\partial x_i\right)$, assuming the eigenvalues have been ordered.
- [Discussed problems associated with vector field topology methods (discriminant, second invariant) to characterize the topology of the flow]. For shock accelerated inhomogeneous flows, Q criteria produce the best results. Region identification schemes share some common problems (global threshold issue, hard to quantify strength, comparison, direction, interaction and evolution of vortex).
- Looking now at the vortex core line versus the vortex region - with vortex core lines an accurate construction of vortex structure is made possible. What is the relationship of the velocity vector and the three eigenvectors? This is a key question. Most of what we are learning is coming from the visualization community (with some exceptions). But, current existing coreline algorithms failed in the (presented) RM simulation and produced misleading results.
- At Fluent we are now building a software infrastructure for tracking a variety of flow features (extraction, tracking and quantification). (Showed example of the FloWizard CFD software).
- To summarize, accelerated inhomogeneous flows serve as a rich environment for study. Accurate identification of vortex and vortex corelines is important to understand both the topology and the morphology of this environment. Due to the insufficiencies of existing algorithms we are looking into some new approaches.

Pullin – Going beyond point measures of structures is important because point measures have no sense of coherence. The vortex coreline is a good idea but it assumes that the vorticity is infused. Have you thought about extraction algorithms that can identify shifts?

- In terms of vorticity shifts we are talking about when shear-produced vorticity overcomes location-specific vorticity. We are limiting the scope somewhat but I fully agree with your point.

Wai Sun Don (for David Gottlieb), Brown University, *High Order Methods for Hyperbolic Conservation Laws*

We will demonstrate that spectral and other high order methods can be applied to shock problems. We will argue that high order information is contained in the calculations and a proper post processing can yield high order accuracy away from the shock. Results on R-M will be shown.

Wai Sun Don, Brown University, *Space-Time Adaptive Multi-Domain Hybrid Spectral-WENO Methods for Nonlinear Hyperbolic Equations*

The fine scale and delicate structures of physical phenomena related to turbulence demand the utilization of high order methods within performing numerical simulation. Spectral methods are well known for spectral accuracy for approximating analytical functions by expanding the functions in terms of some appropriate basis functions. Owing to its non-dissipative, non-dispersive and conservative nature of the methods, spectral methods are an efficient and high resolution numerical method for computing solutions of PDE that contain both large and small scale structures as in turbulence simulation. However, spectral methods produce O Gibbs oscillations if solutions of the PDE at any time become discontinuous as evidenced in the shocked solution of nonlinear hyperbolic PDE. Various reconstruction techniques such as the inverse and direct Gegenbauer reconstruction have been developed in the last ten years to address this issue with various degrees of success.

On the other hand, high order WENO finite difference methods have been shown to capture the discontinuities with essentially non-oscillatory nature while maintaining high resolution in the smooth regions of the flow field. The WENO methods, however, are more dissipative and computationally more expensive than other similar though lower order shock capturing methods (PPM, for example). Many researchers attempted to address these two issues by hybridizing the WENO methods with various other finite difference schemes. By computing the inviscid fluxes in the smooth regions by faster, less dissipative and less dispersive fine difference methods (Compact scheme, optimized or standard Central difference scheme), the hybrid algorithm improves the efficiency and resolution in the smooth regions and captures the discontinuities with the WENO fine difference scheme. The regions of the high gradient and discontinuity are usually determined by comparing the gradient of the solution at each grid point with some pre-set tolerance. This procedure of estimating the smoothness of the solution $O(\Delta x)$ at best. It is not sufficiently accurate for computing the gradient of function with high frequency components and often leads to application of an inappropriate type of algorithm in such regions.

In this talk we will introduce the recently developed hybridization of the spectral methods and the high order WENO finite difference methods for the discontinuous solutions of non-linear hyperbolic Conservation laws in an adaptive multi-domain framework. The main idea is to conjugate the non-oscillatory properties of the high order WENO scheme with the high computational efficiency and accuracy of spectral methods. Built as a multi-domain method, algorithm adaptivity is used to keep the solutions parts exhibiting high gradients and discontinuities inside a WENO subdomain while *the smooth parts of the solution remain inside a Spectral subdomain. A high order version of the multi-resolution algorithm developed by Harten is used to determine the smoothness of the solution in each subdomain to obtain its overall smoothness structure. Under such framework, the Gibbs phenomenon can be avoided since Spectral methods will not be used to perform approximation of discontinuities, which in turn would allow one to bypass the use of post processing techniques. Improvement in the efficiency and resolution can be expected as well.*

- Unfortunately David Gottlieb is not able to attend the Symposium so I will give both his talk and my own. I will introduce the spectral method, and then I will discuss approximation theory and linear hyperbolic equations with discontinuous solutions and non-linear hyperbolic equations. I will discuss spectral methods for discontinuous solution and discuss a Weighted Essentially Non-Oscillatory Scheme and focus on the multi-domain hybrid spectral-WENO model containing hybrid algorithms. The model work is still in progress.
- First, a brief overview discussion of spectral methods. Error approximation depends on how smooth the function is. If the solutions are discontinuous (as with shock) we have the Gibbs phenomenon. This is magnification of the slow decay of the coefficient. (Discussed conditions for approximation to enable recovery of spectral accuracy and presented several theorems).
- Turning now to solving a PDE using the spectral method. [Presented several theorems. Discussed pseudo spectral approximation of the wave equation. Discussed ways to stabilize the pseudo spectral method for the variable coefficient case (essentially creating a low pass filter)].
- Turning now to nonlinear equations. The spectral method is unstable (as it is in the linear case). Using the spectral viscosity method we add a high order term to the right-hand side to provide artificial damping of high viscosity.
- (Discussed the Pseudo Spectral algorithm approach, including details of time stepping scheme, mapping and filtering). The advantages of using mapping include reduction of round-off error and reduction of the spectral radius of the differentiation matrix. (Discussed several reconstruction techniques).
- [Provided brief explanation of WENO method and Richtmyer-Meshkov instabilities (RMI)]. (Presented plots of convergence study with varying interface thickness and density using spectral and WENO methods. Showed comparison of Spectral and WENO3, WENO5, WNO9 and WENO11 schemes for interface density).

Woodward – Is the remnant of the initial condition right?
Comment – There is no "right."

Woodward – Does the WENO approach steepen things artificially?
- No, what you are seeing is a remnant from the initial condition. If there is a "good" initial condition then that will not be there.

Woodward – These two solutions do not appear to agree.
- (NOTE – there seemed to be some disagreement among the Symposium participants about whether the graphics for the approaches agree well).
- (Showed spectral method graphic for high Mach number).

- So, we have a spectral method (that is particularly good for high resolution) and the WENO method (that is good for capturing shock). Can we put some methods together? We know that others have tried (Caltech for example).
- We partition the domain into a number of sub domains (of equal size). In the smooth regions we use the spectral method and then we use WENO for high order flow and shock. We do this in 1D and 2D. The solution changes with time so we must be able to change the domain from spectral to WENO and WENO to spectral. At each time step we check a series of requirements to determine whether we should stay in spectral or go to WENO (or vice versa). For adaptivity we need to know key information such as interfaces between the sub domains, the smoothness of the solution in a given sub domain and relevant gradients. To address the issue of smoothness we employed the high order resolution (wavelet) analysis.
- (Showed graphics/movies of combined spectral-WENO method in both 1D and 2D).

Pullin – With respect to comparison between WENO and spectral – so far as we know in multi dimensions the Euler equations are ill-posed -- so there is no convergence. The solutions do not exist. We are trying to model systems that have real regularizations (such as viscosity).

- The low order method has too much dissipation to reflect the evolution of the small scale. The higher order method buys you something (if it is real).

Livescu – How do you know how much dissipation you need?

- Only enough to stabilize (no more).

Zabusky – One expects phase reversal with heavy/light. There are some features we are used to – how do you look at this? My first impression is of an indentation of the phase reverse spike and then an even structure feeding into the phase bubble. Could you answer the questions about the features (that are not usual at lower Mach numbers)? What are the features caused by? The wave you solved the shock problem? Going back and forth between the two methods?

- We find some of the same features if we use just the WENO method.

Paul Woodward, University of Minnesota, *Towards an Improved Numerical Treatment of Turbulence in Astrophysical Flows*

We have recently developed a subgrid scale (SGS) model for compressible turbulence for use in our PPM gas dynamics code. This model is implemented in the code and is being validated against data from a simulation of Mach homogeneous, decaying turbulence that was carried out on a 2048^3 grid using our PPM Euler code. The key feature of the turbulence model is a model for the rate of energy transfer to unresolved turbulence from the larger scale flow. This model was motivated by our analysis of data from a simulation of Richtmyer-Meshkov instability carried out on an 8-billion-cell grid with our sPPM Euler code in 1998. This analysis revealed a strong correlation between the energy transfer rate to turbulence and the local flow topology, as quantified by the determinant of the deviatoric, symmetric rate of strain tensor. We have since confirmed this correlation in other flows, including the 2048^3 homogeneous turbulence simulation we are using to validate the new turbulence model. Essentially, the correlation implies that energy tends to be transferred to small *scale turbulent motions when the flow field is compressing in one dimension and expanding in the other two (as happens when you clap your hands) while energy tends to flow in the other way when the local flow field is compressing in two dimensions and expanding in the third (as happens when you squeeze a tube of toothpaste). The full model will briefly be explained, the methods for validation using very highly resolved Euler simulations explained, and initial results presented.*

- ❖ I would like to discuss a new model that I have been putting into my PPM code. This turbulence model is designed for astrophysical applications (there are no walls in astrophysics, no hard surfaces, 95% of the universe is gas). I am thinking about turbulence generated in the gas. I would like to see whether by putting a turbulence model into PPM I could gain some advantage. Examples that have motivated this are convection in stars (like tornadic storms) and jets from protostars or galactic nuclei. The goal is to see – if I put in a physically motivated model for small scale turbulence – can I come out ahead of computing small scale turbulence with the Euler method? (Showed PPM simulation of AGB star convection on a 1024^3 grid).
- ❖ There are lots of turbulence models available. What is different about this one? We have been in the business of running large calculations and this model is based on extremely large simulation data sets. We reference simulations performed with Eulerian code. (Showed 1998 volume rendering of a thin slice calculation with 8 billion grid points). We identified the energy exchange rate from large scale to small scale modes – we find sign reversals in the energy transfer rate. Because of the symmetry (which we did not originally want) we find a "central fountain" with a positive energy rate at the top and a reverse sign at the bottom. We plotted various things that might be associated with this energy exchange rate (enstrophy and symmetric strain rate tensor). What is different between the positive and negative energy areas? We found differences in forward transfer (akin to clapping one's hands) and inverse transfer (akin to squeezing a toothpaste tube).
- ❖ The RM flow may be rather special – can we try to find it in a numerical experiment? We began with Mach 1 with well-resolved perturbations and expected to see certain things. We find that we are doing some things wrong and would like to know whether putting a turbulence model into the code will fix some of the problems.
- ❖ (Discussed the transition of the filtered momentum equation and the subgrid-scale stress tensor to the equation for the time dependence of the subgrid-scale kinetic energy in the co-moving frame). It is important to write this in the co-moving frame (turbulent kinetic energy must be Galilean and variant). [Showed graph of fit to forward transfer – when looked at two times (halfway through and all the way through) and with filtering]. We can measure the decay as turbulence turns into heat. We use the 2048 "chunk of turbulence" to initialize problems.
- ❖ The real test is to put this all into a model (and we did). [Showed a movie half way through (t=1.10)]. I should expect the model to tell me where there is (and is not) turbulence. Grid size was selected based on the time needed to do the run (256^3) – we just finished the turbulence model last week so we did not have a lot of time to prepare it for this talk. (Showed graphic from PPM simulation of Mach 1 decaying turbulence on a grid of 256^3 cells at t=1.10 and comparison graphic with grid of 2048^3. Some large scale structures are coming through. Showed graphics with PPM with SGS turbulence model at same grid sizes]. In principle there are no knobs in this turbulence model (which can be unfortunate if you want to make it work).

- What about turbulent kinetic energy? Introducing the turbulence model provides a new variable turbulent kinetic energy. (Showed compensated velocity power spectra at t=2 for PPM and PPM LES simulations of decaying Mach 1 turbulence on different size grids).
- [Showed problem used to test the turbulence model – introduced circulating flows in the third dimension (to flip sign for energy rate). Showed graphic of vorticity magnitude with (and without) turbulence model]. What I do not know is whether there is difference (other than aesthetic) between the kinetic energies of small-scale turbulence graphics. But I intend to find out.

Pullin – What does the model add for strain rate tensor?
- There are two pieces, the latter being what we use to quantitatively measure the sign flip.

Comment – A standard test for SGS model is to look at the decay rate of kinetic energy. Have you tested this with your 2048^3 model?
- We see turbulence decaying at difference times.

Zabusky – There is a boundary you do not have in your flow.
- What we did was motivated by a single fluid but we got the idea from the RM concept. We put in a factor of density to make the units right. I think that I would look closely at each time we added a rho and consider whether we should do something else (when we go beyond a single fluid case). This does not attempt to model the energy-containing scales. What if I put in Mike Steinkamp's turbulence model that diffuses the interface? That is going to inhibit the formation of little vortices that could be resolved. My putting in the turbulence model has inhibited the growth of those vortices but I need to do this at different resolutions. The model assumes a scale separation (that we all know is wrong).

Clark – Recent work on eddy viscosity suggests that the backward transfer may not be a localized phenomenon.
- There is a problem that I did not discuss with this model. The way I transfer the energy is with eddy viscosity (and that can be negative). What does that do? The answer is nothing (and I find that vexing). Was it helpful to have removed the last factor of $2\Delta x$ and have put it into the dynamic model? I do not yet know the answer to that.

Zabusky - Recently I read a paper on RT that was published in JFM last year. The author does not deal with the problem of the density gradient interface. This is a multi fluid code (2 species) and the author invents a process and term to address momentum transfer. I think this is going to be very important in RT.

Comment - I think you are applying the KH to a different physics issue.
- The idea was to take the classic 2D shear layer thought to be the progenitor of turbulence and make it 3D - as the instability itself develops half of the sinusoidal wave form is where the fluids are coming at each other and the determinant turns on. Rollers or no rollers - if we perturb in 3D - this will turn on. Half the time (statistically about 1/3 the time) it is doing anti-diffusion. I do not think there is a bug. Perhaps there is not really any energy. I view this as a numerical experiment – if the mechanism for transferring the energy is to remove it locally and I

put it into the smooth variable – then this is what I get. Perhaps I should be taking it out of larger modes and put it into little random noise at smaller wavelength. We have not yet defined a relative figure of merit for this as representation.

Comment – This is an important point for the physics as well as the numerics.
❖ I need to refine the grid more and determine whether I see these little rollups. If you have figures of merit to propose - I would like to hear them.

Comment – What if you take a hypothetical, idealized reaction with reaction rate as a function of time asymptotically - as far as you can? That is a figure of merit.
❖ I have looked a bit at how others validate their models and have so far not found much that I think would be useful. It is fairly clear what the model is supposed to give. If anyone has suggestions, I would welcome them.

Comment – For incompressible flow the two figures of merit vary significantly. One test is channel flow (although you do not have boundaries) – this has both computation and experiments.
❖ Again, I have no walls. A wide channel with a focus on the center might be relevant.

Holm – We modeled and found it required the 2048^3 and resulted in 11 Terabytes of data (which is available to anyone who wants to look at it).
❖ A natural thing is to debug one of the flows we have been using at scale. I have always said that PPM is second order and converges linearly (for a nonlinear problem). We threw out a lot of higher order things that do not make any difference (they were expensive).

Comment – We have heard about some simulations using very high order schemes. Does the order matter?

Zabusky – I have looked at WENO calculations in the literature. Very high increase in order often does not show up in RT at very short times. I am not sure what is going on.

Comment – The main thing is not order but resolution.
❖ I think there is a definite relationship between order and doing a better job - but I think the relationship is weak.

Comment – When doing a shock the order becomes less important.
❖ What we should all be doing at $2\Delta x$ is damping.

Comment – Climate codes are spectral because they do a good job at delivering wave numbers to the right place at the right time.
❖ I compared PPM advection with a high order climate code and found no real difference. One can find very high order codes that are not very good (but there are no low order codes that are very good). I think there is a point of diminishing returns in the smooth areas (where PPM does some fancy things). There is no part of these flows that will stay smooth forever without a wave coming by.

Glimm – In the discussion of numerical accuracy I think fluid and numerical interfaces are far more damaging than shocks. There is a large difference in the degradation and the errors tend to couple into the physics. I think we should be talking interface methods (rather than orders of accuracy). Bill Rider and Doug Kothe have determined that the untracked methods are the worst and there is a hierarchy among the interface methods. No one has mentioned numerical surface tension, for example, and this tends to be very important. The interface methods are a more appropriate topic of conversation than the order of accuracy (2^{nd} order give 80% of what one is likely to ever get).

Bhimsen Shivamoggi, University of Central Florida, *Spatial Intermittency in Compressible Isotropic Turbulence*

Theoretical formulations are considered for spatial intermittency in compressible fully developed turbulence. Multi-fractal formulations in the inertial and Kolmogorov-microscale regimes are given. Compressibility effects on the dissipation anomaly are discussed.

- ❖ I will discuss spectral laws for the inertial range and then discuss equilibrium statistical mechanics and spatial intermittency.
- ❖ One effect of compressibility is the exchange of compressive kinetic energy and the internal energy of the fluid. Another effect is that energy is radiated in the form of sound waves. This sound energy must ultimately be converted into heat by the various processes of acoustic attenuation. Numerical simulations showed vortices that are most intense near the shock waves.
- ❖ I take a first cut and add a compressibility parameter. Scale-invariance arguments applied directly to the Navier-Stokes equations in conjunction with the scale-invariance condition on the kinetic energy dissipation rate yield the spectral law. The mean kinetic energy dissipation rate changes under the scaling transformation.

Holm – Do you know about Chuck Leith's scaling model?

- ❖ I know Chuck. I will talk with you later about more details.
- ❖ The kinetic energy spectrum in the compressible case is steeper than that in the incompressible case. This appears to be due to the coupling of vortices in the sound waves. One may take a heuristic approach and make *ad hoc* assumptions about the stochastic nature of the local mean kinetic energy dissipation rate and determine the effect of this feature on some of the original local similarity arguments.
- ❖ Multi-fractal models are based on the idea that a singular measure result from a self-similar multiplicative fragmentation process has a limited scale invariant distribution. The compressible FDT is assumed to posses a range of scaling exponents. Observe that compressibility effects tend to reduce intermittency corrections.
- ❖ (Presented detailed equations for addressing spatial intermittency in compressible fully developed turbulence. Discussed the importance of degrees of freedom in fully developed turbulence.) Observe that compressibility effects reduce the number of degrees of freedom (this is traceable to the development of coherent structures revealed by the DNS of compressible FDT). Experimental data on incompressible 3D FDT suggested that the singularity spectrum function around its maximum may be expanded up to second order via the parabolic-profile model. I have shown a way to take the Kolmogorov forward for the spectral case.

Xiaolin Li, Stony Brook University, ***Improvement, Simplification and Extraction of the FronTier Code and Its Applications to Fluid Interface Instabilities and Other Scientific Problems***

We describe significant improvements to the Front Tracking package, especially in the 3D handling of topological bifurcations. We also assess the performance of the package, in comparison with publicly distributed interface codes (the level set method), with published performance results (VOF and other methods) and with previous versions of front tracking. The major new algorithm presented is Locally Grid Based tracking (LGB), which combines the best features of two previous 3D tracking algorithms. It combines the robustness of grid based tracking with the accuracy of grid free tracking and is a significant improvement to both algorithms. We also discuss the surface curvature and normal algorithms and a higher order propagation algorithm, used for comparison studies.

- I want to begin with a brief discussion about the basics of the front tracking method. I wanted to debug and compare the details of our code with other interface methods so I will present our work over the past couple of years.
- Front tracking is not widely used in the scientific community. To have Lagrangian (front tracking) methods we have to simplify the interface for users (and that is another component of our work). The front tracking method (separation of domains into sub domains) was introduced by Richtmyer in the 1950s and originally designed for fluid dynamics. In the 1980s Jim Glimm showed that this method could be used for the tracking of instabilities. The front tracking method divides space into sub domains, propagates the front and uses finite difference (volume) for interiors. The evolution of the geometrical interface drives the complexity of the front tracking into higher resolutions (3D).
- Major issues for FronTier include accuracy of propagation, accuracy of geometrical calculations, optimization of interface mesh, robustness of topological bifurcation (this became a saving point for the level set method), coupling interface-interior solutions and simplification for users (this is important if the front tracking method is to become a prevalent approach in the scientific community).
- I will now compare the front tracking method with the level set and other methods. I will discuss recent developments for the front tracking method and the application of front tracking to CFD and other scientific problems.
- There are two types of front propagation: point (the velocity of the front is independent of interface geometry velocity field) and surface (Runge-Kutta). [Discussed details of a comparison between front tracking and the level set method (point Runge-Kutta)]. I looked at first order comparisons at fifth order level set (WENO) versus fourth order front tracking (Runge–Kutta) and also looked at other comparisons. I found that all of the methods failed the problems I used (including deformation reversal test) except the Marker Point method (Rider and Kothe, 1995). I also looked at 3D interface velocity reversal tests. I also compared with the VOF method (Kothe, 2005).
- (Discussed comparisons for both point and surface propagations). To perform Runge-Kutta it must be applied to the entire surface and the order of accuracy must be accompanied by the

matching order of accuracy in calculation of geometry variables. My objective is to bring the front tracking method to second order accuracy. With 3D I encountered significant problems with robustness in topological bifurcation.

- (Discussed comparison between locally grid-based (grid free) tracking and grid based tracking). Recently we have created an approach that combines the strength of both – we call it the locally grid-based method. We use the grid-based approach to do topological bifurcation – this is a compromise between my work and work completed by James Glimm.
- I do not have time to talk about the coupling of the interface and interior.
- [Showed some applications of the front tracking method (R-M, R-T, thin film, MHD, fusion pellet, forest fire propagation, simulation of leukocyte cell migration)].
- I want to make the front tracking method easy to use and easy to understand. In my future work I will focus on simplifying the user's ability to use the code.

James Glimm, Stony Brook University, *Modeling and Simulation of Turbulent Mixing in Real (Nonideal) Fluids*

Turbulent compressible Rayleigh-Taylor mixing displays experimentally self-similar mixing and universal growth rate properties, but simulations do not show universality. We report on a new class of simulations (based on a new front tracking algorithm and on inclusion of real fluid effects) with agreement to experiment within 5%. Comparing solutions with distinct numerical methods (and differing numerical mass diffusion), we find variation of the growth rates by factors of two or more. Comparing ideal to real fluids in simulation gives a variation of the growth rate by 30%. Comparing different tracking algorithms changes the growth rate by 20%. Our conclusion is that modeling of turbulent mixing is sensitive to details of transport, surface tension, and of course a transition to turbulence, and to their numerical analogues. These facts have implications for the development of a predictive model of turbulent mixing, which will be discussed.

- There are two basic issues I will address in this talk: (1) simulations of fine scale turbulent mixing and (2) multi-phase mixture models (enabling one to do larger scale systems). These two issues are related because one validates the models by looking at the microphysics (DNS) simulations.
- I am talking about scale-breaking phenomena (both physical and numerical). These are important and make macroscopic changes in the result. [Story – calculation of RT alpha is controversial and we have traditionally been known for being higher than experimental data. We managed to fix our numerical methods and our results got worse (our data got higher). The second thing we did was to add more physics and now we have 5-10% agreement with lab experiments for R-T mixing. To the best of my knowledge no one has achieved this before].
- I am talking about acceleration driven mixing (mostly RT, some RM). We are interested in the penetration distance of the light fluid into the heavy fluid. The alpha becomes most important for describing the macro behavior of the mixing process – we have found that alpha can vary by a factor of 2 or more when looked at from the perspective of scale-breaking phenomena. (Showed Rayleigh-Taylor simulation for weakly compressible, immiscible fluids (with surface tension).

- Now I will discuss removal of numerical non-ideal effects (numerical surface tension and mass diffusion), adding physical non-ideal effects (surface tension, mass diffusion, compressibility), validation against laboratory experiments and analyzing data and validating closure relations in averaged equations against DNS simulations.
- Turbulent mixing – most computations under-predict mixing rates relative to experiments. The cause for this appears to be numerical mass diffusion, which reduces the local density contrast and thus the large scale mixing rates. Questions are raised about the role of initial noise in the experiments.
- Numerical non-ideal effects include mass diffusion (can be removed by tracking, errors modify density contrast by a factor of 2X for typical grids), numerical surface tension (reduced by local grid based tracking, errors proportional to curvature that arise from approximation of interface by a line segment within each mesh block.
- Physical non-ideal effects include compressibility (the solution depends on initial temperature stratification and to compensate we use a data interpretation with a time dependent Atwood number to restore self similarity - but the mixing alpha rate increases with compressibility).
- How to develop the time dependent Atwood number? (Discussed details. Showed graph with comparison of tracked and untracked (incompressible) simulations. Showed graph with renormalized definition in which alphas (theory, experiment, simulations) come to closer agreement).

Zabusky – Are you going to change the saturation of your curve?
- This is an older simulation that contains numerical surface tension.
- Now I will talk about recent improvements to Front Tracking and new turbulent mixing simulations – we eliminated surface tension and added more physics – we are now in agreement within a 5-10% range for immiscible and miscible fluids. The two ideal fluid calculations show a factor of 3X discrepancy due to combined effects of numerical surface tension and numerical mass diffusion.

Zabusky – It would be helpful if you would plot $\dot{h}$ (as has been done in a recent JFM paper).
- (Showed table with comparison of experiment with two numerical methods with (and without) surface tension and with (and without) mass diffusion). The simulations are consistent on three different measures of mixing rates.
  - To simulate the miscible experiments we allow controlled diffusion across a tracked interface. (Showed graph with two time steps and domain size of 5 cells (explained that this is the typical length scale in the middle of a complicated RT simulation before getting to the next bubble).
  - (Discussed the grid based error analysis (origin of numerical surface tension issue).
  - Diffusion is more common as a scale-breaking parameter than is surface tension. Different experiments (with different dimensions, materials, conditions) may have different dimensionless diffusion. None will agree with numerical diffusion unless by accident. Dimensions vary greatly from one experiment to another.
  - Turning now to use of accurate DNS simulations to averaged equations (now validated against experiment). [Discussed process for two phase equations and approaches for deriving p*, v* and (pv)*]. We have data now available for analyzing closure hypotheses (discussed example of three way comparison). The closure hypothesis appears to do well.

Further work will assess closures against simulation data, assessing simpler closures and a variety of closure hypotheses.

Woodward – There is an immiscible phase with Euler above and Euler below. What happens when the front that is being tracked wants to develop curvatures?

- ❖ The interface will not get infinitely complicated (it will be a little more resolved than the grid spacing). I think numerical surface tension prevents overly high curvature.

Zabusky – This is an important issue and should be a focus for discussion in the general discussion.

Ray Ristorcelli, Los Alamos National Laboratory, *Initial Condition Dependence of Rayleigh Taylor Turbulence*

A lattice Boltzmann methodology is used to study the initial condition dependence of RT turbulence. The simulations are for non-mixing, variable density with Atwood numbers A=0.3 – 0.6. Initial conditions with both deterministic and stochastic modes are studied. It is found that the amplitude of the initial interfacial perturbation is not as important as the mean zero crossing rate, or equivalently, the initial Reynolds number, of the interface. In addition the time to transition of the flow and the asymptotic growth rate is strongly influenced by the nature of the stochastic modes of the initial condition as the unresolved perturbations in an LES it is seen that the unresolved modes substantially affect the flow's evolution. This is discussed in the context of current LES capabilities and future LES developments.

- ❖ Here are the points I would like you to take away from this presentation:
  - ➢ Point 1 – 2D computations are not relevant to 3D flows.
  - ➢ Point 2 – the nature of the small-scale fluctuations affect the flow.
  - ➢ Point 3 – the existence of small scale fluctuations affect the flow even if the large features (single mode) are resolved.
  - ➢ Point 4 – A single parameterization of the initial interface by its thickness cannot capture the growth rate.
- ❖ We are dealing with variable density, RT turbulence (not compressible). We are using a constant g force. We are interested in looking at LES and other approaches (versus more true physics). There is a background noise that may be thought of as the unresolved noise one might see in a large eddy simulation. Computations run until the edge of the RT layer hits the edge of the domain. This is a work in progress. [Discussed nomenclature for single deterministic mode and noise, flow and turbulence metrics (layer width, alpha parameter, Reynolds numbers – bulk and turbulent, turbulence intensity and production dissipation ratio). Showed center line slices from a 3D single mode simulation with noise. Showed 3D pictures showing evolution of 3D RT layer. Showed several sets of simulations with modes and noise varying. Showed comparison of 2D and 3D single sinusoidal mode simulations (with and without noise)]. Looking at height of the layer there is a 50% difference in 2D versus 3D. There is no similarity between 2D and 3D for the turbulent Reynolds number. The turbulence intensity at the center line is very different in 2D versus 3D. The alpha growth rate factor comparison shows that the 3D alpha is not asymptotic (2D is).

- Now looking at interfacial perturbations (showed concentration on the center plane, heights (increasing wave numbers of initial conditions delay transition, increasing initial conditions amplitude produces a minimal effect). We find some interesting things on this comparison that warrant further study. Turbulence intensities appear to scale (within an order of magnitude) with the aerodynamic growth rate. Production dissipation plots show very bizarre results.
- Moving now to a single deterministic mode with varied noise. The take home message is that there is a big difference between noise and no noise. There is no conclusion on turbulence intensity. The alpha growth rates do not appear to be hitting an asymptotic regime (finer scales appear to produce a faster long term growth rate). The production dissipation ratio settles into some consistency. The last set of simulations also shows a delay in transition. We see different behaviors for the turbulent Reynolds numbers. I cannot offer a key concept that brings all of these graphs together to explain what is going on.
- In summary –
  - For 2D versus 3D – 2D physics have nothing to do with 3D physics (big difference). 2D computations will not capture 3D physical flow.
  - Noise only – in the absence of large scale features the nature of the noise is important.
  - The evolution of large scale 1D features in the presence of noise – there is a big difference between noise and no noise (this presents a problem for coarse grid scale simulations). Noise makes a nominal difference so long as the zero crossing rate of the initial conditions is about the same (the zero crossing rate is determine by the large scale features). The noise makes a difference to the turbulence itself (if it does not make a difference to the large scale parameters of the flow).

H. Pitsch, Stanford University, *Large-Scale Integrated Multi-physics/Multi-code Simulation of Aircraft Codes*

The presentation will focus on two aspects of computational modeling. First a new consistent model for premixed turbulent combustion using a level set method to describe reactive fronts will be presented. Different aspects involve the discussion of the physical interactions of turbulence and a premixed flame, LES filtering of fronts, the models for turbulent burning velocity, the numerical methods for accurately describing the evolution of level sets, and the application of the methods in complex geometry flows. In the second part, large-scale integrated multi-code, multi-physics simulations will be presented. The example of a LES/RANS coupled simulation of the compressor and combustor of an aircraft engine will be shown and the integration environment will be discussed.

- At Stanford we have an ASC Center that is tackling a large scale fully integrated simulation of the full aerothermal flow through a gas turbine engine (showed graphic with components of engine being simulated). Different parts of the engine are governed by different physics so we use different codes (which have different models) that must be coupled together. We use a fully compressible formulation in the RANS code and a low Mach number formulation for the combustion chamber. We need to couple these together and be able to describe multi-physics issues. Verification and validation of large-scale integrated simulation is a significant challenge.

- ❖ Today I will focus on modeling for premixed combustion in the context of LES (we have density jumps in thin layers and other similarities to problems that are being discussed today). I will discuss filtering techniques for interfaces and surfaces. The basic assumption is that chemistry is fast but not infinitely fast. If there is an equation with two terms that balance one another they cannot be modeled independently. (Presented and discussed a regime diagram for turbulent premix combustion LES).
- ❖ What are challenges for LES? Flamelet models often involve solutions of reactive scalar. Flame is thin compared to the filter scale (there is a discontinuity that one needs to resolve). Reactive scalars typically jump within one cell from unburned to burned value. A numerical solution is not possible with conventional methods. We solve for a level set function G (which has no jump across the interface). Then we can write an equation for the evolution of the level set (across one front) - the definition of G-equation away from the surface is arbitrary.
- ❖ The Flamelet front moves by convection (not important to this discussion) and by interaction between the curvature and the transport region that leads to flame propagation. Larger scales of the turbulence can only "wrinkle" the flame (they are too large for the preheat region).
- ❖ Earlier today we heard that it is complicated to solve level set equations accurately. We need to come up with criteria that we can use to assess whether a given numerical simulation is sufficiently accurate. For validation we have looked at difference meshes (fully hex, fully tet) and comparison with experiments.
- ❖ Turning now to the integrated simulations – we couple solvers (each has been enhanced with a subroutine to check where it needs to connect to other solvers). Every time we have a new code release this can be a hassle so we have developed a coupling environment (that talks to five different codes simultaneously) and we use that to tie the level set solver into a code and to get the solvers to talk with each other.
- ❖ There is also the issue of boundary conditions (LES to RANS and RANS to LES). [Showed simulation of PW compressor-combustor flow field (LES to RANS)].

Clark – Are these all in the same time step?

- ❖ Yes, there has to be a common clock somewhere. In conclusion I want to point out that if something is happening in a turbulent flow on the smaller scale it is important to understand the interaction and to understand at what scale the interaction takes place.

Ristorcelli – Are there any simple test cases that you can use to predict extinction, etc?

- ❖ For non-premixed combustion we know what to look for and there is good data. But, for premixed combustion that is not the case. At this point I do not think we really know what quantities we need from the experiments (and experimental data is scarce).

Question – Would there be an advantage to looking at simple laminar flames?

- ❖ No, this goes beyond laminar flames (and we know we can do laminar flames). The simulations that I showed today are based on full chemistry on laminar flames.

Second Chances & Round Table: *Heinz Pitsch, Wai Sun Don, Shuang Zhang, Norman Zabusky, Bhimsen Shivamoggi, Ray Ristorcelli, James Glimm, Paul Woodward, Xiaolin Li*

Pullin – For Jim Glimm who made the statement that the scale-breaking phenomena impacted the alpha parameter. This has broad implications.

Glimm – Dimensionless scale-breaking parameters are time dependent (they differ by roughly a factor of 10). I do not fully understand everything that is out there but scale-breaking clearly has a profound effect.

Dimonte – Another question for Jim Glimm – Have you tried a simulation in which you ramp up gravity from zero and then ramp it down again?

Glimm – No, we did not do that. If there is enough interest then we might run experiments with time-dependent gravity.

Ristorcelli – Even if you do not have to have something to compare it to – just running the simulation would help us to suggest experiments.

Question – Would you explain further your approach to closure?

Glimm – Take the Euler equation and multiply by the characteristic function of one of the fluids – get a new set of equations and most of the terms will be reinterpreted as a density of each phase so you end up with twice as many equations and twice as many variables. The analog to Reynolds stress is an additional term. We can test things numerically and eventually have to make assumptions (a physics postulate) and can get to some closure. You get a lot of new parameters and it can get ugly. Our approach has fewer phenomenological parameters – the main parameter is the growth rate of the mixing zones.

Christon – The typical thing done for closure is to say that all materials in a cell see a uniform rate of strain. Is that there?

Glimm – No, this is a complete, first-order, mixed phase closure. It is whatever you can possibly get from first order closure.

Zabusky – Local entropy generation before it becomes turbulent in a flame?

Pitsch – There was a study that looked at - if you have heat release, how does that influence turbulence. It turns out to influence the turbulence on the smaller scales (not the larger scales) so it is captured in LES (and we get away with not modeling it). It depends on the filter size. Someone did an experiment taking turbulent jets and looking at structures, then introducing fuel and there are no structures. People said it was because of viscosity but the experimenter found the local Reynolds number to be the same and still the structure is different – we do not model this.

Zabusky – I have problems with front tracking. I first heard about it from Jim Glimm at a Gordon Conference many years ago. I asked what one does when the interface gets very long. He told me that we clip it – I think there is a lot of massaging going on in front tracking. What if the vorticity (if it is being generated by front tracking) is on the interface and you clip it? You have gotten rid of a lot of entropy.

Pullin – Does clipping add dissipation?

Zabusky – Clipping is just removal.

Glimm – In our opinion what is added is numerical surface tension and the recent improvements help that (but do not eliminate it). Surface tension inhibits small scale structure. Numerical mass diffusion is not the same as physical mass diffusion either but it is a good analog.

Zabusky – I would like us all to agree on is the value of plotting the enstrophy. The initial condition determines a lot (especially if we do not go asymptotic). Why not plot the enstrophy during the initial condition? It does not cost anything and it may provide a better handle for what is going on than some other options. The next question I have is this – we all talk about the interface (front tracking, G) but what is the gradient at the point of the interface? Is it wide or narrow? What is the steepness of the gradient at the point we call the interface? I think this is important. The stretching causes the gradient to get smaller but when you stretch a vortex layer you limit the KH flexibility. You cannot only talk about the interface - you must also talk about the gradient.

Glimm – The surface tension of the gradient is at a molecular level in the two simulations we ran.

Comment– I can see that by front tracking you are setting up a boundary condition and you would expect strong shear.

Glimm – We allow independent variables for the velocity. We are not enforcing a common tangential velocity.

Ristorcelli – I would like to ask the audience a general question – would it be embarrassing to compute the enstrophy? Is it something that we have any confidence in? It is the smallest scale feature in some of these flows.

Comment – If you are doing DNS you are resolving everything (including enstrophy).
Ristorcelli – There is DNS in theory and DNS in practice. They are not always the same.

Comment – If you are doing LES then my understanding is that enstrophy is dominated by the small scale. With LES it would be a non-computable property (you might be able to model it). If you have a sufficiently good SGS model then you might model it but the SGS model must be capable of doing it.

Comment – And there has to be the assumption of a cascade.

Zabusky – Enstrophy is enstrophy – you don't have to have a model. If the notion of enstrophy is problematic then change it from enstrophy to circulation (especially at the beginning).

Ristorcelli – When you add smaller scales there is more dissipation that is taking place right away and it takes more time for the buoyancy to act.

Zabusky – At the beginning a dominantly vortexed process is taking place. Before things become very turbulent (just prior to the upward turn in transition) – I think you would be rewarded if you look at the integrated vorticity along z. In the Andrew Cook, William Cabot and Paul Miller JFM paper that I referred to earlier there is one picture and it contains the only mention of vorticity in the whole paper. My point is that I believe the region is vortex-dominated and strongly influenced by initial conditions.

Holm – That is hard to do if you are doing DNS. I think vorticity is always useful. I have not seen Rayleigh-Taylor afficionados look at enstrophy.

Clark – I will briefly comment on that tomorrow.

Zabusky – I think plotting H dot (rather than H) would be more revealing.

Ristorcelli – What do you look at to say that region is vortex-dominated?

Comment – He has no Reynolds number.

Zabusky – Another way of doing this is with molecular dynamics (I know this is being done at Los Alamos National Laboratory). What is going on? The Kadau 3D simulation (showed on screen) shows the bubbles closing up – how could this structure form? I believe that the structure forming at this time is associated with a vortex.

Glimm – I can tell you what happened. You have two RT spikes and they fall into each other.

Zabusky – Have you diagnosed the vorticity?

Glimm – If you look at the density plots then you can see what is happening.

Zabusky – It is possible there is vorticity elsewhere.

Glimm – I know there is because I have seen this many times.

Zabusky – I think looking at H dot is another way to look at the problem. I would like to interpret this flow as a vortex reconnection (and have done so but I do not have a response to the paper that has been written discussing this yet). I believe it is the dominant thing at this particular time.

Glimm – Malcolm Andrews' work supports your point that something could be gained from doing that.

Holm– The potential flow model is driven by vortices.

Glimm – The dominant physics is in the buoyancy-drag equations (and that is an ODE). Vorticity is one part of a big picture that has many other aspects.

Zabusky – The large-scale structures are playing an important role. The simulation may not be big enough.
Comment – I agree. The simulation is never big enough.

Livescu – I agree that this is an important topic - we should look at the structure of the mixing layer as well as the growth of the mixing layer.

Thursday, August 4, 2005

Victor Calo, University of Texas – Austin, *Residual-Based Multiscale Models for Large-Eddy Simulation of Turbulence*

Variational multiscale concepts are used to construct subgrid scale models for Large Eddy Simulation (LES) of turbulence. The basic idea of this framework is to introduce an a priori decomposition of the solution into coarse and fine scales. The coarse scales are identified with the numerical approximation, while the fine scales are identified with the subgrid scales and need to be modeled. A residual-based fine-scale approximation is proposed by extending to the nonlinear realm algebraic approximations of the Green's function. These approximations, based on the theory of Stabilized Models, may be thought of as the modeling component of the proposed approach. This new modeling concept is very different from the classical LES modeling ideas, which are dominated by the addition of eddy viscosities. Applications of the approach are presented.

- I will discuss a slightly different approach to what has been discussed up till now. We do not think that a spectral method is the ideal approach – we are working on schemes that attempt to approximate the effects of the fine scales onto the resolution. First I will discuss incompressible Navier-Stokes, then I will discuss LES, and I will offer some examples and conclusions.
- (Discussed details of incompressible Navier-Stokes equations). LES is designed to solve a problem that has varied scales. We simulate the coarse scales to be our numerical solution and use fine scales for what we cannot resolve. (Discussed variational space-time formulation equations and variational multiscale formulation). The completion of the space, with respect to the coarse scales, is the fine scales. (Discussed a new variational multiscale method). Assume in the coarse scale problem that we have fine scales (and in the fine scales that we have coarse scales). We introduce approximation for the fine scales and assume the fine scales are the solution for the coarse scales. We try not to use viscosities, we come up with approximations for the fine scales and introduce the approximations into the coarse scales - that is our numerical scheme.
- (Discussed localized small-scale equations and the assumptions underlying their use to obtain an exact solution for the small scales). Our inspiration comes from Stabilized Methods – we evolve an algebraic approximation. Once the approximation is introduced we have our model. (Discussed a comparison of this approach with classical stabilized methods). This can be thought of as a nonlinear stabilized method. This approach does not need eddy viscosity. (Discussed the application of the model to bypass transition problem).
- I will now discuss isogeometric analysis. The main tenet is to obtain exact geometry on even the coarsest meshes. The basis functions used are Non-uniform rational B-splines (NURBS). We decompose the mesh into NURBS patches and index parametric space. We then refine the mesh using analogues of h- and p- methods and a new k- refinement. (Showed the application of this analysis to turbulent channel flow ($Re_t = 180$), hydroacoustics (Eppler 387 airfoil) and fluid-structure interaction).
- In conclusion we have developed a small-scale approximation which precludes the use of eddy viscosity. We believe that isogeometric analysis provides exact data transfer from coarse to

finer grids and the geometry and solution are naturally preserved across mesh refinements. We have seen robust performance of discretization schemes - we can achieve good convergence using GMRES with diagonal preconditioning and ILU.

Zabusky – Do you have any experience comparing with the reverse boundary method?
- ❖ No, we have compared with a momentum preserving scheme.

Question – Did you use a pressure smoother in your finite volume calculation?
- ❖ The scheme uses constant pressure.

F. Grinstein, Los Alamos National Laboratory, *On Implicit LES for Turbulent Flows*

Large Eddy Simulation (LES) is an effective intermediate approach between DNS and RANS, capable of simulating flow features which cannot be handled with RANS such as significant flow unsteadiness and strong vortex-acoustic couplings, and providing higher accuracy than RANS at reasonable cost but still typically an order of magnitude more expensive. In the absence of an accepted universal theory of turbulence, the development and improvement of subgrid scale (SGS) models has been unavoidably pragmatic and based on the rational use of empirical information. Classical approaches have included many proposals ranging from, inherently-limited eddy-viscosity formulations, to more sophisticated and accurate mixed models, e.g., [1]. Their main drawback relates to the fact that well-resolved (discretization independent) LES becomes prohibitively expensive for the practical flows of interest at moderate-to-high Re. Recently, many researchers have abandoned the classical LES formulations, shifting the focus directly to the SGS modeling implicitly provided by non-linear stabilization achieved algorithmically, through use of a particular class of numerical schemes, or based on regularization of the discretization of the conservation laws, [2]. Most numerical discretization schemes can potentially provide built-in or implicit SGS models enforced by the discretization errors if their leading order terms are dissipative. However, not all implicitly implemented SGS models are expected to work: the numerical scheme has to be constructed such that the leading order truncation errors satisfy physically required SGS-model properties, and hence non-linear discretization procedures are required. The analogy to be recalled is that of shock-capturing schemes designed under the requirements of convergence to weak solution while satisfying the entropy condition.

Non-oscillatory finite-volume (NFV) numerical schemes can likewise be viewed as relevant for nonlinear implicit LES (ILES) of turbulent flows [3], if we propose to focus on two distinct inherent physical SGS features to be emulated near the cutoff: 1) the anisotropy of high-Re turbulent flows in the high-wave-number end of the inertial subrange region (characterized by very thin filaments of intense vorticity and largely irrelevant internal structure, embedded in a background of weak vorticity); 2) the discrete nature of laboratory observables (only finite fluid portions transported over finite periods of time can be measured). This leads to requiring that ILES be based on numerics adaptive to the local flow physics (sharp velocity-gradient capturing capability), and using a (conservative) FV formulation. In the MILES approach (recently reviewed in [4]), the effects of the SGS physics on the resolved scales are incorporated in the functional reconstruction of the convective fluxes using locally monotonic FV methods; other proposed ILES approaches are *discussed in [2]. Tests in fundamental applications ranging from canonical to complex flows indicate that MILES is competitive with conventional LES in the LES realm proper (flows driven by large scale features). Use of the modified LES equation as framework for theoretical ILES analysis, suggests that the leading discretization "error" terms introduced by NFV schemes provide implicit SGS models of mixed anisotropic type [3] and regularized motion of discrete observables [5].*

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- What is ILES? (MILES?) – Historical perspective and motivation. I am going to discuss the historical perspective and motivation for using ILES. This leads to the issue of how we capture physics with numerics. There is no free lunch – one must put work into the numerics. I will discuss some of the canonical test cases one needs to use to certify a numerical method.
- DNS – solution for all scales without further assumptions is prohibitive for most practical flows of interest. LES is - practically speaking - what we can afford.
- LES assumptions and issues – we are supposed to look at fairly high Reynolds numbers so the inertial range is involved, the large scales are resolved, and the smaller scale features are modeled. How do we do something with unresolved scales that does not dominate the resolved features of the flow? How does one decide whether the method is good or bad? From a numerical perspective we use the original equation plus source terms (which have to do with particular numerics). The modified equation provides the effective differential equation satisfied by the numerical solution by the given method. It reproduces the original ODE and includes the implicit SGS models. I will focus on compressible LES equations. There is a low pass filter in process and then there are numerical choices (finite volume, element or difference discretization). Then you write modified LES equations in which a number of terms appear as source terms (explicit GSG stress model term, commutation error term and discretization "error" term). The well resolved LES requires that the last term should be negligible. The problem is that one cannot usually afford to have the last term negligible (because it is too expensive for a real life problem).
- (Discussed details and best uses of LES functional models and structural models). Overall conclusion? Non-conventional SGS modeling approaches need to be explored. Alternative LES methods focus on convectively dominated dynamics, dealing with under-resolution, regularization, and weak solutions. Implicit LES fits in the framework of an alternative LES.
- Implicit LES uses a finite volume framework and has no explicit filtering (so the commutation error term can be dropped). A minimal SGS model will be used so the resolved and unresolved scales are uncoupled.
- If we base our numerics on a stable (consistent) framework then ILES converges to DNS to the same extent expected from any LES. When based on NFV numerics, ILES is competitive with classical LES in the LES realm proper (convectively dominated flows driven by large scale features).

- Not all implicit SGS modeling will work. Shock-capturing schemes provide an analogy (this is, deal with weak solutions and make sure that all basic physics laws are satisfied). We have to build the physics into the numerics.
- Bill Rider has developed a nice history of LES – and found that there are some things to learn. The first shock capturing approach and the first LES have the same basis, for example. Shock capturing methods and LES evolved similarly (particularly their ability to evolve with the flow features). Physical requirements for nonlinear implicit SGS models include adaptiveness to local flow physics and sharp velocity-gradient capturing. Another key component is conservative finite scales in space and time. This suggests that we should work with finite equations of laboratory observables. That means numerics that are capable of looking at observables and able to adapt to local physics. Other desirable requirements are dissipative relevant solutions, nonlinear stability and positivity (where needed). Methods developed for shock capturing essentially have these features.
- A short history of implicitly implemented SGS modeling begins with local monotonicity preservation (MILES) and includes work on engineering, astrophysics and geophysics. The modified LES equation is used as the theoretical framework for ILES. The lead discretization error terms introduced by NFV schemes provide implicit SGS models. MILES has been used extensively for free and wall bounded flows. [Discussed application of MILES to turbulent channel flow problem and recent validation studies on the Taylor-Green vortex case (transition to turbulence and decay)]. One thing to keep in mind is that one is essentially changing the Reynolds numbers of the flow when one changes the grid.
- This approach is a natural extension of shock capturing concepts for compressible turbulent flow. You are trying to capture the small scale vorticity organization and the inherently discrete nature of observables. The modified LES equation provides the theoretical basis for ILES.

Pullin - I accept that shock capturing methods can be viewed as SGS models for shocks. When you are using an explicit model there are parameters that one must work hard to compute dynamically. It happens that the modified equation has the right parameters to act as a SGS model. That is surprising.

- There are knobs. Each method has its own qualities. Some schemes are less diffusive at the lowest order and achieve better agreement with the DNS. There are knobs (features of the numerical schemes) that have to be tuned. We have to build the physics into the numerics (and we have to learn how to do this).

Woodward – There is 30 years of technology that has gone into these schemes and that is not trivial. Perhaps some of the details do not matter. Although there are a few key ingredients that one must have for shocks one appears to be free to do a number of different things because certain details do not matter. We have just not thoroughly verified that they do not matter.

- You have to become clever and think carefully about the problems you are trying to address. The nice thing about this method is that the competition between the numerics and the modeling is minimized because you are concentrating on only one thing. You will likely have to add explicit models to address other things.

Pullin - I think you have made progress. It is surprising that the truncation errors are going to have constants that will adjust what is needed for a SGS model.

Darryl Holm, Los Alamos National Laboratory, *Introduction to LANS-Alpha, the Lagrangian Averaged Navier-Stokes Alpha Model of Turbulence*

We used Taylor's hypothesis of frozen-in turbulence to derive Lagrangian-averaged (LA) fluid equations with constant Navier-Stokes (NS) viscosity and constant correlations length (alpha) of a Lagrangian trajectory with its mean. These LANS-alpha equations provide a closure model for either compressible or incompressible turbulence.

Lagrangian averaging follows fluid parcels and modifies the nonlinearity in the motion equation while preserving its Lagrangian invariants, such as circulation integrals for the inviscid part of the flow. Lagrangian averaging is nondissipative: it preserves nonlinear coherent structures that are bigger than its mean correlation length, alpha. Taylor's hypothesis imposes closure by assuming that excitations smaller than alpha are swept along by the larger circulations, instead of diffusing them.

We analyzed the viscous incompressible solutions of the LANS-alpha equations for existence and uniqueness in three dimensions using standard methods going back to Leray. We found that they possess a global attractor whose fractal dimension is finite and bounded as $Re^{3/2}$. *This bound implies enhanced computability, relative to NS, because LANS-alpha reduces the number of active degrees of freedom at sizes smaller than alpha. This is seen as a steepening of the kinetic energy spectrum E(k) which changes from* $k^{-5/3}$ *to* k^{-3} *for* $k\alpha>1$*, caused by the modified nonlinearity in the LANS-alpha equations. Viscosity then enters to balance the modified nonlinearity at wavenumber* $k\alpha \sim Re^{1/2}$ *in agreement with the* $Re^{3/2}$ *estimate of fractal dimension. This mechanism for reduction in the number of degrees of freedom also holds for compressible flows. We also tested the LANS-alpha equations for their effectiveness in modeling turbulence, by: (1) comparing their steady solutions with mean experimental data in pipe flows, for physical realism at high Reynolds numbers, (2) comparing their direct numerical simulations of forced turbulence with corresponding results for NS in periodic domains, for relative speed up and proper numerical solution properties and (3) comparing results with alternative models, especially with the "dynamic model" in large eddy simulations of turbulent mixing layers, for speed and accuracy. These new turbulence models are now being implemented at the subgrid scale parameterization in the Los Alamos Parallel Ocean Program for high resolution global ocean circulation.*

- I will discuss deriving CLANS-alpha equations in 3D. C is for compressible, LANS is for Lagrangian-averaged Navier-Stokes. Here are a few properties of the LANS-alpha model:
  - It produces explicit LES-like models by regularizing NS
  - Imposes Taylor's hypothesis on fluctuation dynamics
  - Analytically provides existence, uniqueness and convergences of LANS-alpha solutions to NS solutions as alpha goes to zero
  - Has a global attractor
  - Shows good agreement with experimental pipe and channel data at highest experimentally available Re
  - Computational work scales as Reynolds squared (not Reynolds cubed)
  - It enslaves the small scales to the larger scales when the small scales get smaller than alpha

- This approach easily allows the addition of compressibility
- The turbulence community uses two kinds of averaging (Lagrangian means and Eulerian means) and their commutation properties differ. One must be careful of the order of the spatial derivative and the Lagrangian mean.
- Alpha models are second-order turbulence closures for a known set of generalized Lagrangian Mean (or GLM) equations. They introduce a length scale (alpha) that is the correlation length between an exact Lagrangian trajectory and its mean trajectory. The Lagrangian-averaged EP variational principle produces Eulerian equations, which are non-dissipative.
- The LANS-alpha model is a GLM fluid model that is closed by Taylor's hypothesis (sweeping of fluctuations by mean flow) and an *ad hoc* viscosity. GLM averages are Eulerian quantities (discussed equations and details). Discussion of Taylor's Hypothesis closure (linearize fluctuation relations, assumption of flow rules) and examples of applications (including discussion of properties that should be part of the barotopic motion equation such as vortex dynamics, momentum density, dissipation of energy.
- The 3D CLANS-alpha may be interpreted as a Compressible Large Eddy Simulation (CLES) model.

Pullin – When you add *ad hoc* viscosity, is it the true viscosity?
- There are two forms of energy and at some point you have to resolve the dissipation. The filter width (alpha) with the Taylor hypothesis (scales smaller than alpha swept by the larger scales) and the time for cascading is constant if K is smaller than minus three.

Pullin – When one goes to compressible flows it is unusual to solve global Helmholtz equation.
- This has been successfully implemented by thinking of the global inversion as a local filter.

Woodward – LES literature describes a subgrid model but all of the literature appears to describe a sub filter model.
Comment - I find that a sub filter model is easier to deal with conceptually than a sub grid model.
Pullin – I do not understand implicit filtering. My understanding of the sub filter model is that the various filtering processes destroy information near the cutoff and the sub filter information tries to restore that information (up to the cutoff). That is, one restores the destroyed information up to the cutoff by filtering whereas the sub grid models attempt to conceptually evaluate the dynamic effect of the unresolved scales on the resolved scales. I find the two difficult to separate conceptually.

Dale Pullin, Caltech, *Large Eddy Simulation of Richtmyer-Meshkov Instability with Reshock*

We will discuss results obtained from large eddy simulation (LES) of the Richtmyer-Meshkov instability with reshock off an end wall. The numerical method is a hybrid (weighted essentially non oscillatory) scheme coupled to a tuned, centered-difference (TCD) method (Hill & Pullin 2004). The simulations were performed in a unigrid environment at a maximum resolution of 776x2562. The subgrid scale (SGS) model is the stretched-vortex model of Misra & Pull (1997). WENO is activated in thin regions containing shock waves, but reverts smoothly to the TCD scheme away from shocks where turbulence is present and where the SGS model is activated. Several *configurations of shocks initially traveling from light (air) to heavy (SF6) have been simulated to match experiments of Vetter and Sturtevant (1995) and good agreement is found in the growth rates of the turbulent mixing zone. The stretched-vortex SGS model allows for subgrid-continuation modeling in which we match large and small scales at the resolved-scale cutoff and estimate the contribution to certain statistics from the unresolved portion of the flow. This multiscale modeling extends flow anisotropy from the resolved-scale to the dissipation-scale range. It also provides estimates of the subgrid scalar variance, which in turn enables calculation of the full probability distribution function of the mixture fraction of air/SF6, including the contribution of subgrid scales and the effect of Schmidt number.*

- I will discuss LES methodology, the hybrid WENO-TCD computational method and our attempt at "multi-scale modeling". (Review of Richtmyer-Myer Instability) – the vorticity generation is the important term. There are applications in astrophysics and ICF. (Discussion of flow description and conditions in a shock tube). We are trying to model the experimental window of observation that focuses on the reshock. (Discussed Favre-filtered Navier-Stokes equations). The explicit SGS model is a stretched vortex model that was designed originally to model turbulence at fine scales. We make the assumption that inside the grid cell the subgrid motion is represented by a vortex that has some internal structure (and some number of the vortex internal properties need to be known). [Discussed model parameters (subgrid energy spectrum, parameters obtained from resolved-scale velocity structure-functions, subgrid vortex orientation).] The model can be used to calculate many properties of the fine scales of turbulence (showed example of scalar spectrum from stretched spiral vortex).
- The numerical method is a hybrid scheme known as WENO-TCD (similar to what Wai Sun Don described yesterday with a few differences) that uses a five-point stencil and second order accuracy. At shocks (only) the method reverts to full WENO. The optimal WENO stencil is matched to the TCD stencil. The algorithm has been well tested in 1D, 2D and 3D (example of Riemann 1D wave). It is a filter-free computation.
- Carlos will discuss some AMR extensions of this method in his talk. I will focus on the main run (Case Vie; 776 x 256 x 256) – (showed three images of the growth of the turbulent mixing zone). Various statistical measures of the instability and its evolution are studied (for example, kinetic energy in the mixing layer). We measure various turbulence statistics (for example, plane-averaged turbulent Mach number and sound speed). The mixing layer behaves almost incompressibly.
- The stretched-spiral vortex SGS model is used for subgrid continuation. We can compute the plane averages of various spectra (radial velocity, for example). We can use the subgrid to get an idea of the PDF of mixture fraction with subgrid correction.
- Building a hybrid method that would work and be suitable for shock capturing and LES turned out to be more difficult than originally expected. Our idea of multi scale modeling is to try to estimate the subgrid contribution to some of the statistics

Holm – Would you discuss the dynamics for the sub grid orientation?
- It is an algebraic rule. An alternative would be to think about subgrid vortices and that can be done – it provides an extra set of equations to solve. This is an algebraic rule – in a region of pure strain the structures would want to align with the principle eigenvector of the resolved scale.

Holm – It would be exciting to see your dynamics emerge as if there were subcell-dynamics of the submerged vortex.

Zabusky – With respect to the growth of the turbulent mixing zone – is there a simple way to calculate the growth rate?
- ❖ If it were not for the expansion the result would be different. The expansion reinvigorates the growth – this may (or may not) be fortuitous.

Clark – How to get an estimate on k (subgrid scale kinetic energy)?
- ❖ To get subgrid energy I integrate the subgrid energy spectrum equation (Lundgren) from cutoff to infinity. I have all I need to compute the local subgrid kinetic energy.

Woodward – You have the SGS kinetic energy – have you made a picture and compared that? Since you have a resolution study the lowest resolution run should agree with the resolved kinetic energy on the high scales – do those agree?
- ❖ We have done coarse comparisons of subgrid scale energy and resolved energy at various resolutions – but this is not quite what you are saying.

Woodward - Your model produces a natural spatial distribution.
- ❖ That is an interesting idea.

C. Pantano, Caltech, *A Low Numerical Dissipation, Patch-Based Adaptive-Mesh-Refinement Method for Large Eddy Simulation of Compressible Flows*

The numerical simulation of compressible turbulent flows often necessitates local mesh and scheme adaptation. This can be accomplished naturally by applying a single grid solver with numerical flux evaluation depending on the locally dominant physics embedded into a block-structured mesh adaptation. We will describe a hybrid finite difference solver for large eddy simulation of compressible flows that is shock capturing, exhibits low numerical dissipation away from shocks and is integrated into the block-structured dynamically adaptive framework AMROC (adaptive mesh refinement object-oriented C++), the core of the CFD efforts of Caltech's ASC Alliance Program. The scheme is designed for the simulation of 3D compressible turbulent flows driven by shocks. We will describe the flux-based approach that remains discretely conservative during dynamic scheme switching and at fine coarse interfaces resulting from structured mesh adaptation. In smooth flow regions, a centered discretization tuned to capture high wave number dynamics is applied (TCD). A weighted essentially non-oscillatory (WENO) method is used for shock capturing and has been modified to transition smoothly to TCD in shock free regions. The method is a development and significant improvement of the hybrid scheme developed in a unigrid context. Several verification and validation simulations will be discussed. The results range from one to three space dimensions and include homogeneous shock free turbulence, turbulent jets and the strongly shock-driven mixing of the Richtmyer-Meshkov instability.

- Dale's talk focused on the physics and I will discuss more of the numerics associated with the hybrid method. We work with an AMR infrastructure as our main data structure. There are benefits to both structured adaptive mesh refinement (SAMR) and LES for compressible flows. Unfortunately there are mutually exclusive numerical needs of shocks and turbulence (shock capturing methods around discontinuities, low numerical dissipation methods for LES in turbulent regions). There are also (fairly standard) theoretical and performance issues associated with formulation, choosing between schemes, conservation, convergence, accuracy, stability, minimizing dispersion errors at scheme boundaries and fine-coarse mesh interfaces.
- Our current infrastructure is based on Berger and Colella's algorithm for conservation laws. Boundary conditions and synchronization between patches is accomplished by filling ghost cells with interpolated data. We can do this because most SAMR patch solvers use numerical methods that are dissipative.
- If we have a few levels of refinement then time interpolation does not provide much but with many levels of refinement time interpolation can provide savings. The interfaces are called hanging nodes – to make them conservative a special correction (known as fix-up) is applied.
- We use implicit boundary representation with signed/unsigned distance function (arbitrary triangulated implicit surfaces handled by closest-point transform algorithm). AMR refines close to the fine pieces of the solids (resolving thin structures with AMR).
- What are the challenges of SAMR to LES? First we need to change the patch solver (and that can be done easily although one has to be careful at the boundaries). There are two possible changes to the SAMR data structure – one minimal and the other massive. Minimal involves no changes to the data structure and communication whereas massive requires that changes be made consistently throughout mesh interfaces. The choice of the temporal integration scheme is far from trivial.
- We use Favre averaged LES equations in conservation form –this is important when dealing with shocks because it ensures weak convergence. We assume that the SGS model depends parametrically on the cutoff scale and that it varies slowly and continuously in space. There is no filtering performed.
- Tuned-Centered Difference (TCD) is implemented in flux form. We use stable energy conserving boundary stencils. There are two possibilities for scheme hybridization (fine grained and coarse grained); we prefer the fine grained hybridization technique. Shocks are handled by a finite difference WENO. Because of fine grained switching we modified the optimal stencil of WENO to match the TCD (switching is somewhat rudimentary at this stage). At mesh boundaries we use WENO fluxes at the mesh interfaces (only on the first cell of the fine mesh).
- The Runge-Kutta scheme has to be changed. We have to change the fix-up because we have multiple stages. Time interpolation and the modified fix-up reduce the temporal accuracy from 3rd to 2nd order at the boundary.
- We have some validation results to report - planar jet, jet flame, RM and convergent shock for turbulence. (Provided details on validation with non reacting turbulent jet experiment, Richtmyer-Meshkov instability).
- We have measured how much time is spent by different parts of the algorithm – 50% of time is spent computing, 50% is spent communicating and interacting. The communication was not optimized for this run on the LLNL Frost platform (now defunct). The code has about a half a million lines. Complex boundaries are not something we have had a lot of experience with.

Glimm – Can you put surface tension on your interface?

❖ We have not considered that because we have been dealing with mixed fluid.

Pullin – It would be hard but I think it could be done.

❖ We have done an exploding cylinder as a benchmark calculation.

Second Chances: *Darryl Holm, Victor Calo, Fernando Grinstein, Carlos Pantano, Dale Pullin*

Holm – A question for Victor Calo. Your projection is onto a finite number of modes (full solution of the PDE). Do you assume your solution has particular properties (you are doing a Taylor series in small quantity) –so, in some norm the difference between your projected solution and the real solution is small?

Calo – We are working on that now. Thirty years of experience in stabilized methods shows that linear functions work fine whereas nonlinear functions do not work as well. We are working on the latter.

Grinstein – Dale Pullin was discussing reservations about truncation error. WENO is a nonlinear numerical method that adapts to the feature of the solution. That is how we can build in physics.

Pitsch – Stanford (Parviz Moin) implemented this WENO model as described in the literature and first recomputed the decay of the turbulence (for isotropic turbulence) and got the same results. Then his team changed two parameters in the FCT and found that it changed the solution. They applied this to compressible turbulence and changed the temperature and saw that the parameters did not hold.

Grinstein – We have had four different people using WENO in four different codes and they all had similar results. All numerical methods have knobs and if you change the knobs you will get different answers. Hopefully one gets to a point that the physics being captured is independent. I think these things are problem dependent but some methods are more robust than others.

Pitsch – The point that - in some contexts the constant is very important - is something we must keep in mind.

Grinstein – The methods are dynamic in a sense because they adapt to the flow. I heard a presentation about this at an APS meeting but I have never seen any evidence of this in the literature. My experience is that with WENO the user must understand how to use the code.

Calo – I used the model and had to tune to get optimal dynamics.

Pitsch – For low Reynolds number DNS the filter rate is a parameter and few will argue with that.

Pullin – The question is this - is WENO a useful MILES method? And, if not, then why not?

Grinstein – I have not used WENO myself.   There would be a basis for comparison.

Rider – I have tried WENO for ILES and found that it does not perform very well. WENO is too dissipative for small scale structures. I have tried 5th and up to 13th order WENO. Resolution is inferior to what you get from schemes like PPM.

Holm – The framework that I showed today was an example that easily accommodates heterogeneity and anisotropy. But the method that Dale showed has more life than what I showed. What I showed would drag with the flow the correlation tensor that would deform with the shear. What Dale showed seemed interesting because it has direction cosines each of which has its own life. Dale's approach fits into the same framework that I described today.

Comment – I know that there is some thinking about extending your ideas to shocks.

Holm – At Stanford there are people working on 1D equations and we have been also working on a pressureless case (capturing the flows between two domains that are different).

Comment – It does regularize the shock profile. The difficulty is in coming up with an entropy condition solution.

Comment – I spoke with Cameron (who is now at the University of Colorado) and he thinks he can make this work on shocks.

Holm – There are several people working on this   If you are running shocks through turbulence and reduce it to 1D and come up with a Berger, is that good or not? What some researchers have found is that if you start with the sine wave and run the 1D version forward it does not go to shock. The big question is should your SGS turbulent model produce a shock?

Question – Would Dale talk about how to get to K to the minus 5/3?

Pullin – There was a hypothesis that at any instant in the evolution you would not get to K to the minus 5/3 – you have to take an ensemble average. These things start out as shapes and if you take an early spectrum you get to K to the minus 2 then they become a tube (K to the minus 1) and the K to the minus 5/3 is a balance. The time step for the LES is sufficient scale at the SGS to get to the K to the minus 5/3. The time scale in which this is evolving is both sub grid scale and sub time scale during a typical LES time scale. I have not explored this in detail (it could be interesting in some applications).

Holm – About handling boundary conditions of the extra variable you discussed (cosine for the vorticity). Do you want it to point into the boundary?

Pullin – That is a good question. We are working on a SGS model for wall bounded turbulence. I do not want the signs to point into the wall but in the directions the streamline vortices point to in the sub layer. Computing the equation that you discussed earlier (direction cosines) must be done carefully to get appropriate physical boundaries. I am not certain how to do that yet. Combustion is an important area for SGS model but I think the wall bounded area is also very important. Currently there is no successful model for treating wall bounded flows.

Zabusky – About the explosion problem that Carlos described- can you handle an intermediate phase where you go to a liquid state before you explode? Can you melt the cylinder?

Pantano – Current we are blasting Al and the tube is flawed.

Malcolm Andrews, Los Alamos National Laboratory, *Opportunities for Direct Numerical Simulation of Rayleigh-Taylor Mix Experiments*

As the speed of computers increases so goes the temptation to perform Direct Numerical Simulation (DNS) of Rayleigh-Taylor (RT) instabilities. Indeed, it may now be possible to compute RT mix to higher Reynolds number than has been achieved in well controlled and diagnosed experiments. However, comparison of DNS with corresponding experiments is fertile ground but one full of mine fields. This talk will indicate the problems we have experienced comparing RT DNS with experiment, and indicate the opportunities that exist to enhance the comparisons and their impact on simulation and modeling.

- ❖ The RT experiment at Texas A&M University (TAMU) is basically a water channel. Distance downstream is converted to time for the Taylor hypothesis. We worked this experiment for 8-9 years and have gathered vast amounts of data as well as turbulence and mixing statistics.
- ❖ Beginning in 2004 we took density and velocity data from the experiment and used it as input for a MILES code (resolution of 128 x 128 x 256). We measured the density fluctuations with a thermocouple and turned them into an initial condition for the computation. We found that the computation did not pick up the high wave number (because of the resolution). We did calculations with initial density only (no initial velocities) and plotted distance downstream (because distance=time). As the mix develops it steadies to a constant valley around 0.7 (which is what we have measured in the water channel for years). We decided that we needed to put in initial velocity fluctuations and – once we did that – we ended up with much better results. That work was completed 2-3 years ago.
- ❖ First some background on the diagnostics available from the experiment. There are thermocouples that allow for measuring temperature and from temperature measurements we can get densities (through water EOS). We can also get PLIF and we have new PLIF diagnostics for the span-wise perturbation. The temperature range is about five degrees Centigrade. Density energy spectra and molecular mixing data are use to parameterize the initial interfacial perturbation in stream-wise direction. The boundary conditions are very anisotropic.
- ❖ We set up the computations with an initial density distribution. The initial potential field is constructed from the measured initial vertical velocity spectrum. In principle all of the experimental data is available at the start of the computation. This is not an easy thing to do.
- ❖ 3D DNS has been performed with initial density and with initial density and velocity conditions. Visualization of averaged density isosurfaces shows initially 2D behavior with 3D structure

emerging later. PLIF density images from the experiment are qualitatively similar to the DNS density field. DNS with initial velocity perturbations grows faster than simulations with only interfacial (density) perturbations. Similar trends in molecular mixing are observed between the experiment and DNS.

- ❖ Most real experiments have density and velocity fluctuations. One needs to be careful about initial conditions (measuring initial conditions in RT experiments is very hard).
- ❖ We are continuing with our comparisons between experiment and simulation at downstream locations for validation, better physical understanding of the transition and model evaluation. More resolution is needed. We are, perhaps, close to a full set of initial conditions for the TAMU water channel. To compare simulation and DNS the experimentally measured initial conditions should be used.

Question – Can you offer a physical reason why the initial conditions affect the acceleration rate?

- ❖ Playing with the initial conditions (density, velocity) one tends to end up with the same result at late time. My suspicion is that long wavelengths (perhaps coming in at late time) may be a factor.

Dimonte –So if your time is long enough the impact of the initial conditions disappears?

- ❖ That is the thinking (but we have not yet proven it). There are many questions still outstanding (what happens to molecular mix at late time?).

Glimm – We have a diagnostic that you could use to assess the extent to which you have eliminated numerical mass diffusion.

Rider – At what time does the simulation change from a DNS to an LES?

- ❖ I don't know the answer to that. We clearly need more resolution. Putting these experiments into the computations is difficult. We have more work to do on the computation. I want you to know that there is an extensive amount of data available to you.

Tim Clark, Northrop Grumman, *Statistics of the Turbulent Rayleigh-Taylor Mixing Layers*

The Rayleigh-Taylor mixing layer poses considerable challenges for both computational methods and turbulence and mix modelers. The presence of sharp interfaces in the density fields, intermittency of the density field, sensitivity to initial conditions and the emergence of larger and smaller scales pose significant challenges to direct simulation and large eddy simulations. Likewise, these effects, as well as the non Gaussian nature of the statistics at the edges of the mixing layer and the phenomenology of the energy and dissipation rate production mechanisms at points away from the mixing pose significant challenges to the turbulence theorists and modelers. These issues will be examined by considering the statistics derived from ensembles of direct numerical simulations of RT mixing layers. In addition, we will examine some of the advantages, disadvantages and needs of both LES and RANS approaches to simulating RT mixing layers.

- ❖ I will discuss some general remarks about modeling and how one might choose to represent flows like RT, if one chooses to use RANS or LES. The RT flow is highly transient. It begins as a stochastic phenomenon with Reynolds number of zero. DNS will not work. One cannot rely on “quasi-equilibrium assumptions” for a lot of this. The flow is highly inhomogeneous (this is a particular problem for the Reynolds averaging approaches). Compressibility may play a strong role at various stages of the evolution. Material strength, heat transfer, phase changes and ionization effects and chemical and nuclear reactions present additional complications.
- ❖ Computational issues include initial conditions (often not known), sharp interfaces (immiscible fluids), rapid development of fine scales [set by a balance of viscous forces and shear induced between the heavy and light fluids on the spike/bubble interfaces (i.e. the sides of the bubbles and spikes)], continuous increase in operative Reynolds number, and, fluctuating pressure induces fluid velocities at points far from the actual mixing layer
- ❖ (Provided graphics showing three realizations) – the initial interfaces look the same to the eye but the bubble/spike structures at late times are clearly not identical.
- ❖ I offer these Statements of Principle:
  - ➢ A high Reynolds number turbulent flow has too many degrees of freedom to fully resolve.
  - ➢ A turbulence model reduces the number of degrees of freedom in a computation (this requires that the model smooth some of the structure or detail of the flow. If the model does not reduce the number of degrees of freedom it is not a useful model).
  - ➢ There is no clear separation of scales in a turbulent flow.
  - ➢ Models cause a loss of detail on the resolved scale of a calculation (we have to learn to live with it).
- ❖ Why do we care about self-similarity?
  - ➢ Real turbulent flows contain far too many degrees of freedom to compute directly.
  - ➢ Mathematical models of these flows are based (implicitly or explicitly) on an organizing principle (such as similarity) that permits the evolution of many degrees of freedom to be described by the evolution of a few. Can the evolution of the fine scales where mixing occurs be described by the evolution of the large scales?
  - ➢ Understanding the organizing principle is a first step to formulating the model.
- ❖ The notion of self-similarity for complex flow geometries is difficult to justify.
- ❖ LES should (in principle) require fewer assumptions about self-similarity (this is probably only true at high Reynolds numbers).
- ❖ Statistical approaches
- ❖ Direct numerical simulations. Represents a deterministic calculation of a single representation.
- ❖ Spatially averaged statistics.
- ❖ Temporally averaged statistics.
- ❖ Ensemble averaged statistics.
- ❖ RANS (Reynolds Averaged Navier Stokes)
  - ➢ The RANS approach implies an ensemble average of realizations.
  - ➢ The goal for RANS models is to describe the evolution of the statistics of an ensemble of realizations – not individual realizations.
  - ➢ RANS approaches are varied.
  - ➢ Engineering RANS models make many tacit assumptions.
  - ➢ What does an ensemble average do? One realization looks lovely. But, as more realizations are added the detail at the interface becomes very difficult to read.

- LES –
  - This is a relatively new field (RANS has been around since the 1890s).
  - Advantages are that one gets the large scale structures and there are relatively few adjustable parameters.
  - Disadvantages are that we must generalize models of the detailed subgrid physics. The large scales may not be deterministic.
  - The LES model assumes that the unresolved scales behave as a dissipative mechanism.
  - Does an LES of a filtered initial condition produce the filtered result of a DNS of the unfiltered state? (Probably not)
  - What statistics should a LES predict? Spatial? Temporal? How should backscatter be presented?

Rider – Do you know what a reasonable SGS model might be that incorporates backscatter and pressure?

- I think that is a good question. I think you have to look at the pressure operator (in the incompressible case). Perhaps someone can answer the question more elegantly.

Oleg Vasilyev, University of Colorado – Boulder, *Stochastic Coherent Adaptive Large Eddy Simulation (SCALES) Methods*

Current large eddy simulation relies on, at best, a zonally-adapted filter width to reduce the computational cost of simulating complex turbulent flows. While an improvement over a uniform filter width this approach has two limitations. First, it does not capture the high wave number components of the coherent vortices that make up the organized part of turbulent flows, thus losing essential physical information. Secondly, the flow is over-resolved in the regions between the coherent vortices, thus wasting computational resources. A novel method for simulating turbulent flows, called Stochastic Coherent Adaptive Large Eddy Simulation (SCALES) is introduced. The SCALES approach addresses the shortcomings of LES by using a dynamic grid adaptation strategy that is able to resolve and track the most energetic coherent structures in a turbulent flow field. This corresponds to a dynamically adaptive local filter width. Unlike coherent vortex simulation (CVS), which is able to recover low order statistics with no subgrid scale stress model, the higher compression used in SCALES necessitates that the effect of the unresolved subgrid scale (SGS) stresses must be modeled. These SGS stresses are approximated using a new dynamic eddy viscosity model based on German's classical dynamic procedure redefined in terms of two wavelet thresholding filters. The results of CVS and SCALES simulations of decaying incompressible isotropic turbulence are presented and compared to DNS and LES results.

- Why is adaptive LES needed? There are multiple reasons. Large eddies versus energetic structures – we do not know *a priori* where the energetic structures exist. Energetic structures can exist at all wave numbers. Non-adaptive LES under-resolves energetic structures, over-resolves in-between and distorts spectral content of a vertical structure by not supporting its small scale contribution.
- Requirements for adaptive LES include an adaptive solver (resolve and track energetic structures, no *ad hoc* assumptions for grid adaptation) and SGS stress modeling (resolving

energetic structures should result in easier SGS modeling, adaptive LES SGS dissipation should be less than LES SGS dissipation).

- ❖ The adaptive wavelet collocation solver is ideal for adaptive LES. The mesh should be a reflection of the physics that are to be resolved. Wavelets are used for bases functions and are localized in wave number and physical space. Wavelets provide both frequency and position information. (Discussed comparison of Fourier modes versus wavelet scales).
- ❖ LES – Use a low pass filter to separate the large scale eddies from the small subgrid scales. Coherent Vortex Simulation (CVS) has a number of advantages over LES (and some potential problems). SCALES incorporates both LES and CVS. (Presented graphics showing SCALES SGS dissipation). (Showed simulation results for CVS versus SCALES and explanation of SGS model scaling). (Presented early results of the Lagrangian local dynamic SCALES model). There are a few problems with this approach so a diffusion term has been added.
- ❖ Future work will be to verify SCALES methodology for realistic turbulent flows, to complement the dynamic model with a stochastic model, to assess the effect of the stochastic model and to extend SCALES methodology to compressible flows.

Ristorcelli – When you do comparisons kinetic energy is one part, but a turbulent Reynolds number is more useful. If you look at trajectories of Reynolds numbers, that could be very helpful.

Alan Kerstein, Sandia National Laboratory, *A Strategy for High-Fidelity Computational Modeling of Flow, Mixing and Reaction in Compressible Turbulence*

The nominal alternatives for representing micro-scale processes within multi-physics turbulent flow simulations are to parameterize them or to resolve them. In fact, a combination of these two strategies is possible, as outlined in this presentation. Namely, micro-scale processes that cannot be resolved affordably in multi-dimensional turbulence simulations can be resolved in some instances using a lower-dimensional formulation at scale not resolved in 3D. A 1D implementation of this sub-grid closure strategy denoted One-Dimensional Turbulence (ODT) is introduced. ODT combines two 1D approaches that have individually proven successful: stochastic iterated maps and reduction of the governing equations using the boundary-layer approximation. Within ODT, sub processes captured by these two approaches are coupled so as to represent both turbulent cascade dynamics and microphysics at dissipative scales, with strong two-way interaction. Model performance is illustrated by representative applications. Progress on implementation of ODT as a subgrid closure for low Mach number 3D flow simulation is outlined. Prospects for extension to compressible flows are discussed.

- ❖ I am going to adopt Darryl's comment from this morning about putting life into the subgrid and use it as a sub title for my talk. The model I will discuss today is somewhat a vision of the future. The proposed modeling strategy combines two conventional cost-reduction methods. We use the mesh dimension best suited for each range of scales. The large scale advection is inherently 3D but flames can be idealized as 1D (local flame-normal coordinate) suggesting 3D for large scales and 1D sub structure in each coordinate direction for small scales.

- ❖ Multi scale spatial representation requires multi-time-scale advancement - 1D resolution scale (small time step) and 3D resolution scale (large time step). The flow state is entirely represented within sub structures; spatial filtering of flow variables is done only for output.
- ❖ First I will discuss what we do to model at the smaller scales. I call this one dimensional turbulence (ODT). ODT incorporates mixing length phenomenology. Unlike other 1D (and 3D) approaches, ODT does not involve averaging. To obtain a turbulence model in 1D apply the boundary layer approximation and either represent advection by diffusion or use a different advection process. On a 1D domain, molecular evolution based on a boundary layer formulation is supplemented by an eddy process. The 1D turbulent eddy amplifies shear; feedback induces an eddy cascade. ODT simulations provide detailed flow-specific representations of turbulence. We develop an eddy rate distribution by assigning a time scale to each eddy. An eddy event consists of a triplet map followed by velocity profile changes. This approach is much like conventional mixing length theory but the concept is applied to all values.
- ❖ Turning now to 3D compressible turbulence simulation based on evolution on coupled ODT domains. This formulation obeys applicable conservation laws, reduces to DNS for flows resolved at scale M and accommodates a level-set method that allows phase reconstitution after fluxing.
- ❖ With eddy viscosity subgrid scale momentum closure instead of ODT this becomes an alternating direction advancement scheme for solving a compressible LES. We have put some life into the subgrid structure.
- ❖ We have completed an ODT near-wall momentum closure for LES applied to turbulent channel flow. To date we have found that it performs reasonably well. An incompressible ODT bulk closure has been applied to decaying isotropic turbulence on a 32^3 3D mesh. ODT captures effects of density variations in a planar mixing-layer application. (Discussed ODT application to Rayleigh-Bernard convection).

Ristorcelli – Can you take means of what you are doing and create an equation for the means?

- ❖ Yes, I can do a closure on eddy viscosity underneath the ODT.

Ristorcelli – So you can see what mean equations look like in this framework. I think that is fascinating.

- ❖ I have also done multi component diffusion. The key is that this is a local mixing length idea. Counter gradient is in there.

Ristorcelli – Can your eddies deform as you move them? Do you allow that?

- ❖ I will define a 2 parameter space to define the eddies and use a yes or no. There are things that could be done for eddy deformation but it raises the dimensions of the parameter space (number of parameters needed to describe an eddy). If one were going to refine by a factor of N then DNS would require N^3 whereas ODT would require 3N.

Bruce Fryxell, Georgia Institute of Technology, *Large Eddy Simulation of Multi-Scale Interactions in Compressible Reacting Flows*

Simulation of turbulent reacting flows in practical systems with sufficient spatio-temporal fidelity is a very challenging task since interaction between chemical and turbulent scales occurs over a wide range. Even in "low" speed flows in gas turbine engines, compressibility needs to be considered since vortex shedding, unsteady heat release and combustor acoustics can couple together leading to combustion instability. Understanding and predicting combustion instability in gas turbine engines is one of the major challenges for which LES using a compressible formulation is necessary and ideally suited. Additional complexity arises when high compressibility effects due to propagation of strong shocks (e.g. scramjet and pulse-detonation engines) or due to real gas (supercritical) combustion (e.g. in LOX-GH2 rocket motors) has to be simulated. Conventional large eddy simulation methods that model the effect of the scales smaller than the grid on the simulated resolved motion fail to accurately capture turbulence-chemistry interactions since combustion process is dominated by small scale processes that are not resolved on a LES grid. Furthermore, all classical numerical methods used for LES are unable to deal with strong shock propagations in turbulent flows without introducing excessive dissipation that eventually overwhelms the physics in the shear layers. Additional problems appear when phase change (due to liquid fuel evaporation) has to be predicted accurately. A new subgrid combustion two-phase modeling approach that has shown an ability to capture accurately the physics of turbulence-chemistry interactions will be describe din this talk. In addition, the development and application of a new hybrid LES methodology that combines this LES approach with a high-accuracy shock capturing technique will be described. Examples of reacting flows in premixed and liquid-fueled gas turbines, supercritical combustion in rocket motors, shock-vortex interactions and detonation in two-phase mixtures will be shown to highlight the capability of the LES solver developed at Georgia Tech.

- LESLIE3D is a well-established DNS/LES code developed at Georgia Tech primarily for aerospace and combustion problems. It has been extensively verified and validated.
- We use a localized dynamic model for subgrid closure of the unresolved momentum and energy fluxes that contains no adjustable parameters. Beginning with the sub grid models, we use LES with filtered equations. There are three subgrid source terms. We close the equations by solving an additional equation for the subgrid kinetic energy.
- We can handle complex flows and geometries. Our subgrid combustion model uses a grid within grid approach (direct simulation of reaction diffusion on 1D lines with stochastic mixing of scalars across LES).
- (Showed some LESLIE3D aerodynamics applications).
- (Discussed hybrid method and its application to Shu-Osher shock problem. Showed some R-M instability applications. Discussed simulation of shock turbulence interaction (non-uniform grid highly concentrated near the shock) compared to DNS data completed by Stanford group).

Zabusky – Your code can handle vaporization? (Answer: Yes) Are droplets the same size?

- They do not have to be. We can handle any size as well as groups of droplets (or individual droplets).

Question – What are the initial conditions for K?
- Constant and very small. The final kinetic energy was around 2000 and the initial was around 1 (just enough to initiate).

Pullin – You said you had no problems switching between two methods?
- That is correct. Presumably one could use this technique with any two methods. If we used different methods we might have different results.

Second Chances: ***Malcolm Andrews, Tim Clark, Oleg Vasilyev, Alan Kerstein, Bruce Fryxell***

Andrews – A "second chance" thought - the gas channel facility at Texas A&M uses helium and air and will be doing work similar to what I described with the water channel. It will be interesting to figure out the density in the mix.

Calo – Have you tried different conditions in your coarse DNS?

Andrews – We pull everything straight from experimental measurements. We can only resolve so much resolution from the experiment. We still have a problem with getting enough resolution down to the smallest scales. We are not picking up the molecular mix profile quite right near the splitter plate, for example. If we can double or triple the resolution then I think we can get to where we need to be.

Ristorcelli – I would like to hear about when these computations do not work.

Calo – We have one calculation that never got to 3D – the problem was with the aspect ratio of the mesh.

Pullin – LES does not work for R_t = 10,000 wall bounded channel flows. There is no accepted LES model that is going to work near the wall.

Vasilyev – Going to higher order sometimes does not pay off.
Pullin – To do flow past a sphere you are looking at a Reynolds number above 100,000. The cylinder is probably just as hard. I think this gets back to the properties of wall bounded flows.

Clark – In the past I had issues with LES because of difficulty in coupling initial perturbations – how to homogenize in a realistic fashion so they produce realistic late stage fields? In the new (aerospace) environment that I am working in LES is the only tool that will work and what is needed are SGS models where we can determine with some degree of fidelity what the subgrid scales are doing. We need to come to grips with a consistent way to address where the small scales are affecting the large scales dramatically (and we need metrics to show we are doing that). Do eddies keep their identity in the same amount of time? You need to know the appearance is right to get the frequency right. I am impressed with what is being done with SGS phenomena but I would like to see some more stringent tests applied.

Question – What do you think about concepts such as unsteady RANS?

Clark – I can imagine an ensemble that can be defined so there is a RANS initial condition with a coherent eddy but at late time you would expect things to become uncorrelated. I do not really see that the URANS - as a theoretical exercise - is self-consistent. I am not sure that URANS makes sense for a lot of situations (wind over a building, for example).

Comment – I used to do URANS. The models that work the best tend to be simpler plume models that sum a bunch of Gaussians obtained from Lagrangian particles. The simplest model that has been around since 1900 may still be the best. You do not really use LES in most practical conditions because you do not know the initial conditions to the extent that you would want.

Vasilyev – People do not pay attention to backscatter – they do clipping. Physically based hybrid models that model frontscatter one way and backscatter another way is what is needed.

Grinstein – How does one decide if a backscatter model is good? Are there any case studies?

Pullin – We did a 256^3 to look at the backscatter issue and we found that the PDF can be broad. We got different results depending on the filter that was used. I think that issue is filter dependent. It is an issue in SGS modeling – to what extent do you model the true PDF? – I think that is probably application dependent.

Question – Have you considered models for backscatter (other than the one you described)?

Vasilyev – If you use global models you do not have backscatter (you have to use local models).

Clark – I think the backscatter is a different form from the frontscatter (which is eddy viscosity).

Comment – Almost all models described are zero equation models and I believe that one-equation models handle backscatter better.

Pullin – Except for the stretch vortex model - that has natural backscatter 20% of the time.

Kerstein – With respect to Tim's point on the RT problem and living with what we cannot resolve – one has to determine minimal dynamics to work from the problem to something an LES mesh can confidently resolve.

Ristorcelli – I have a blob in a RT flow that is subsumed by an LES model. I have a bunch of blobs and my grid size is one inch in size and I have blobs of pure fluid and not pure fluid. I am concerned about the opacity of the medium as well as the EOS and everything in the LES area provides one concentration. LES tells me nothing about blobs. Some of these attempts of SGS statistics are quite old. You have mean quantities – how do you describe the morphology of a fluid in a grid?

Kerstein – If something lives on a 2D mesh – you have to go deep into the modeling world and you cannot necessarily get there from the advancement of the PDEs we are used to.

Ristorcelli – That is why we are leaning towards second moment closure.

Kerstein - You want to know opacity, chemical product, reactions and growth rate. What I was describing as a sub grid structure can be driven by RANS (it does not have to be driven by LES).

Pullin – When Bruce did shock turbulence interaction what are the inflow boundary conditions in the turbulence?

Fryxell - We did decaying turbulence in a box and at some point took that characteristic outflow boundary condition.

Question - Have you done solid propellants?
Fryxell – No.

Roundtable Summary Discussion

Livescu – I would like to ask participants what are some simple problems that could be chosen as canonical problems for RT?

Comment – It is hard to come up with such problems for RT. A good problem is separation (subsonic flow in an expanding channel) – I am not aware of simulations where the separation and reattachment are computed.

Vasilyev – A paper came out of Stanford CTR about five years ago that found a discrepancy of 1% of incoming momentum of the flow that was giving the wrong separation. They fixed the velocity profile and nailed the separation. If you miss the inflow initial condition then it will be wrong.

Comment – My point of view on LES is that it is quick and dirty calculations – not something a theoretically inclined person would look to. LES should be a coarse grid – not the very fine grid (5x DNS resolution).
Pullin – LES started out being about the big scales but turbulence is more than that. I have seen many LES talks where the data is filtered with the same filter used in LES (meaning that the data is processed by the numerical method). I know of no other area in science where I have to process the data by my predictive tool. We should be trying to predict the turbulence with an infinite number of manifestations (many at small scale). The problem should be one of under resolved turbulence simulation (not large eddy simulation). LES has pushed us away from the real focus of what turbulence prediction is all about. You need an approach that continues down to the small scales – something that models the fine scales of turbulence according to what you want that is then coupled to LES. The field needs to get over the roadblock of filtering the data by the numerical method and

declaring victory as the goal of turbulence prediction. It should not be the goal. The relationship between the small scales and the big scales of turbulence is what we should be focusing on. We have too many SGS models *per se* and we should be focusing more on coupling with LES. You need experiments. Rayleigh-Bernard is classic. You want Prandtl number dependence.

Kerstein – There is a clever particle method that reinforces your point – one might have to change the paradigm according to what SGS physics one is interested in.

Vasilyev – The question is how to come up with the right boundary conditions.

Kerstein – Subgrid dynamics problems are also at play in some applications.

Vasilyev – A test problem should never be bounded.

Clark – A droplet flow with chlorine gas going through them at .2 Mach – they are reacting. For us the interest is what is going on in the cell where I have 50-60 drops. That is not an LES problem but I need to know what the LES is communicating at that scale. We found that we need to know the flow rate over the surface – and if we get that wrong – we cannot get the rest of it right.

Acknowledgements

This report is based on the notes collected by Tina Macaluso, SAIC - Advanced Systems Group, during the course of the symposium. The authors would like to thank Tina for her attention to detail, keen listening skills and attentiveness during the workshop. The authors would also like to thank Rob Lowrie for his helpful comments during the development of this report. Finally, we would like to acknowledge Mark Chadwick for providing the funding required to host the symposium.

Appendix I – Symposium Agenda

CCS-2 and ASC Turbulent Mixing & Instabilities Project

Symposium on Modeling & Simulation of Variable Density & Compressible Turbulent Mixing

August 3-5, 2005

AGENDA

Wednesday, August 3

7:00	Taxi pickup Hilltop House, Quality Inn Suites, Holiday Inn Express
7:30 – 8:15	Continental Breakfast
8:20 – 8:30	Opening Remarks
	Chair: **D. Livescu**
8:30 – 9:00	**N. Zabusky** (Rutgers University) Vorticity Deposition and Evolution in Shock Accelerated Flows: Analysis, Computation, and Experiment
9:00 – 9:30	**S. Zhang** (Fluent & Rutgers University) Turbulent Decay and Mixing of Accelerated Inhomogeneous Flows via Flow Feature Analysis
9:30 – 10:00	**D. Gottlieb** (Brown University) Spectral Methods for Compressible Flows
10:00 – 10:30	Coffee Break
10:30 – 11:00	**W. Don** (Brown University) Space-Time Adaptive Multi-Domain Hybrid Spectral-WENO Methods for Nonlinear Hyperbolic Equations
11:00-11:30	**P. Woodward** (University of Minnesota) Development and Validation of a Subgrid-Scale Compressible Turbulence Model
11:30 – 12:00	Break and Discussions
12:00 – 1:00	Lunch

	Chair: **M. Christon**
1:00 – 1:30	**B. Shivamoggi** (University of Central Florida) Theoretical Formulations for Intermittency in Compressible Fully Developed Turbulence
1:30 – 2:00	**X. Li** (SUNY, Stony Brook) TBA
2:00 – 2:30	Coffee Break
2:30 – 3:00	**J. Glimm** (SUNY, Stony Brook) Modeling and Simulation of Turbulent Mixing in Real (Nonideal) Fluids
3:00 – 3:30	**R. Ristorcelli** (Los Alamos National Laboratory) Initial Condition Dependence of Raleigh Taylor Turbulence
3:30 – 4:00	**H. Pitsch** (Stanford University) Large-Scale Integrated Multi-physics/Multi-Code Simulation of Aircraft Codes
4:00 – 4:30	Break and Discussions
4:30 – 5:00	Round Table Discussions
5:00	Taxi pickup returns to hotels, Holiday Inn Express, Quality Inn, Hilltop
6:30	De Colores

Thursday, August 4

7:30	Taxi pickup Hilltop House, Quality Inn Suites, Holiday Inn Express
8:00 – 8:30	Continental Breakfast
	Chair: **M. Andrews**
8:30 – 9:00	**V. Calo** (University of Texas) Residual-Based Multiscale Models for Large-Eddy Simulation of Turbulence
9:00 – 9:30	**F. Grinstein** (Los Alamos National Laboratory) On Implicit LES for Turbulent Flows
9:30 – 10:00	**D. Holm** (Los Alamos National Laboratory/Imperial College) Introduction to LANS-Alpha, the Lagrangian Averaged Navier-Stokes Alpha Model of Turbulence
10:00 – 10:30	Coffee Break
10:30 – 11:00	**D. Pullin** (Caltech) Large-Eddy Simulation of Richtmyer-Meshkov Instability with Re- Shock
11:00-11:30	**C. Pantano** (Caltech) A Low Numerical Dissipation, Patch-Based Adaptive-Mesh-Refinement Method for Large-Eddy Simulation of Compressible Flows
11:30 – 12:00	Break and Discussions
12:00 – 1:00	Lunch

Chair: **D. Pullin**

1:00 – 1:30	**M. Andrews** (Los Alamos National Laboratory) Opportunities for Direct Numerical Simulation of Rayleigh-Taylor Mix Experiments
1:30 – 2:00	**T. Clark** (Northrop Grumman) Statistical Representation of Rayleigh-Taylor Mixing Layers
2:00 – 2:30	Coffee Break
2:30 – 3:00	**O. Vasilyev** (University of Colorado) Stochastic Coherent Adaptive Large Eddy Simulation (SCALES) Methods
3:00 – 3:30	**A. Kerstein** (Sandia National Laboratory) A Strategy for High-Fidelity Computational Modeling of Flow, Mixing, and Reaction in Compressible Turbulence
3:30 – 4:00	**B. Fryxel**l (Georgia Tech) Large-Eddy Simulation of Multi-Scale Interactions in Compressible Reacting Flows
4:00 – 4:30	Break and Discussions
4:30 – 5:00	Round Table Discussions
5:00	Taxi pickup returns to hotels, Holiday Inn Express, Quality Inn, Hilltop

Friday, August 5 – Requires a Q Clearance

TA-3, Nick Metropolis Building, Rm. 1014

8:00	Continental Breakfast
8:30	Talks begin
5:30	End of Session

Appendix II – Symposium Attendees

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